STIC Search Report
EIC 1700

STIC Database Tracking Number: 50345

TO: Dawn Garrett Location: REM 10C79 Art Unit : 1774 April 21, 2005 Case Serial Number: 10/807099	From: Les Henderson Location: EIC 1700 REM 4B28 / 4A30 Phone: 571-272-2538 Leslie.henderson@uspto.gov

Search Notes

Access DB# 150846

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: DAWN GARRETT Examiner # : 76107 Date: 4/17/05
Art Unit: 1774 Phone Number 305 2-1523 Serial Number: 10/807,699
Mail Box and Bldg/Room Location: Remsen 10C79 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

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Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: Organic Electroluminescent Devices

Inventors (please provide full names): JIANMMIN SHI, ERIC FORSYTHE, DAVID MORTON

Earliest Priority Filing Date: 3/23/2004

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search compound shown in claim 1 as part of a luminescent layer and/or device.

thank you.

4

30

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STAFF USE ONLY	Type of Search	Vendors and cost where applicable
Searcher: KH	NA Sequence (#)	STN $780.69
Searcher Phone #:	AA Sequence (#)	Dialog
Searcher Location:	Structure (#) 1	Questel/Orbit
Date Searcher Picked Up: 4/21/05	Bibliographic	Dr.Link
Date Completed: 4/21/05	Litigation	Lexis/Nexis
Searcher Prep & Review Time: 30	Fulltext	Sequence Systems
Clerical Prep Time: 30	Patent Family	WWW/Internet
Online Time: 150	Other	Other (specify)

PTO-1590 (8-01)

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=> d his ful

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L2           659 SEA ABB=ON  PLU=ON  FORSYTHE ?/AU
L3          6888 SEA ABB=ON  PLU=ON  MORTON ?/AU
L4             0 SEA ABB=ON  PLU=ON  L1 AND L2 AND L3
L5             1 SEA ABB=ON  PLU=ON  L1 AND L2
L6             1 SEA ABB=ON  PLU=ON  L1 AND L3
                 D SCAN L5
                 D SCAN L6
L7            17 SEA ABB=ON  PLU=ON  L2 AND L3
                 D SCAN
                 SEL L7 RN

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                D QUE STAT L16

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L29            4 SEA ABB=ON  PLU=ON  L28 AND L26
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L30           86 SEA ABB=ON  PLU=ON  L26 NOT L29
                D L30 1-86 HITRN
L31       667697 SEA ABB=ON  PLU=ON  (LUMINES####### OR FLUORES? OR
                 PHOSPHORES?)/BI,AB OR LED/IT OR PHOSPHOR# OR LUMIN?
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L32 7 SEA ABB=ON PLU=ON L31 AND L30
D SCAN
L33 79 SEA ABB=ON PLU=ON L30 NOT L32
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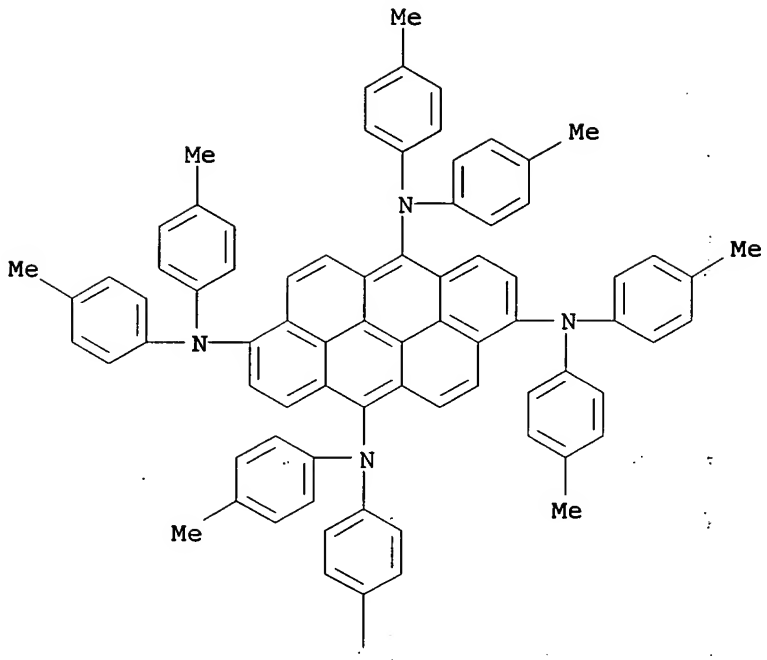
L29 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
2005:182182 Document No. 142:268913 Fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display. Sotoyama, Wataru (Fujitsu Limited, Japan). U.S. Pat. Appl. Publ. US 2005048313 A1 20050303, 25 pp. (English). CODEN: USXXCO. APPLICATION: US 2004-801546 20040317. PRIORITY: JP 2003-305621 20030829.
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

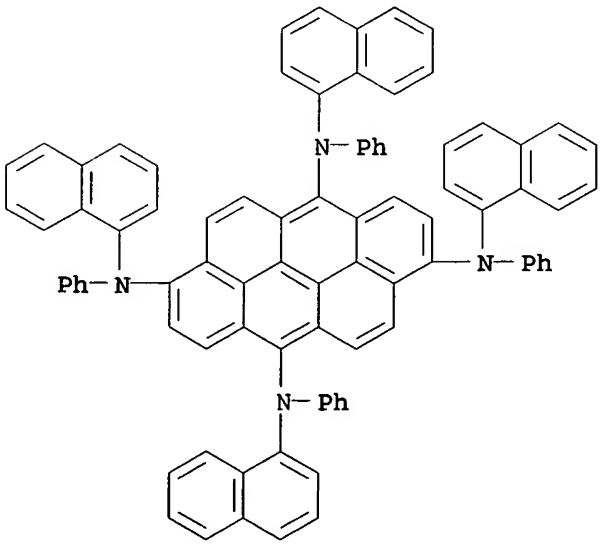
AB The invention refers to an organic **electroluminescent** element having an organic **light-emitting** layer between an anode and a cathode, wherein the organic **light-emitting** layer comprises, as an organic **light-emitting** layer forming material, a fluorescent material comprising a perylene compound I [R1-12 = H or -CH:CH-Ph-N(R13)R14, wherein two or more are not H; R13,14 = (un)substituted aromatic or aliphatic and may be bonded to each other] and/or an anthanthrene compound II [R101-112 = H or N(R113)R114, wherein 4 or more are not H; R113,114 = (un)substituted aromatic or aliphatic and may be bonded to each other]. A fluorescent material that **emits** red **light** with a high color purity and a high luminous efficiency-when used singly or as a guest, an organic **EL** element having a high luminous efficiency, and a high-performance organic **EL** display having a high luminous efficiency are realized.
IT **845896-94-8P 845896-97-1P 845896-98-2P**
RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
RN 845896-94-8 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A



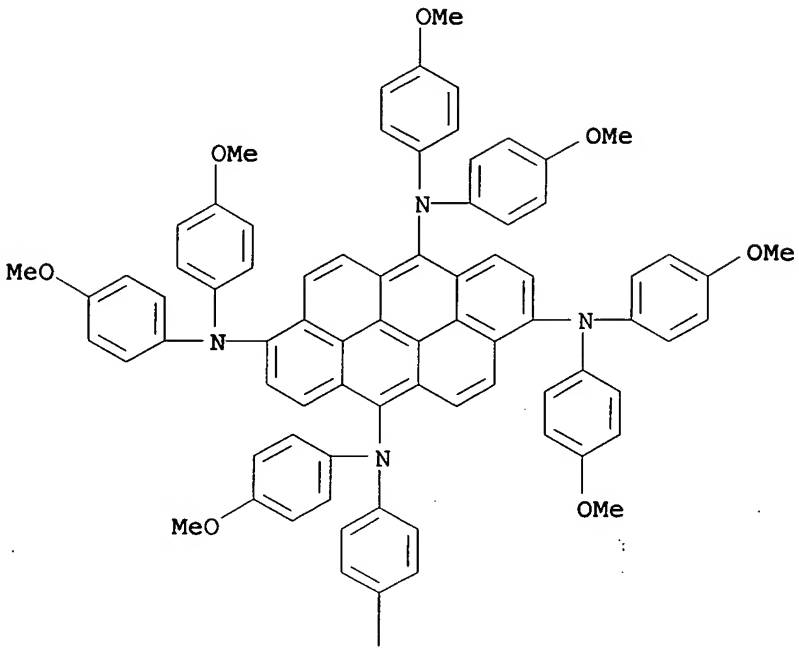
PAGE 2-A

RN 845896-97-1 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



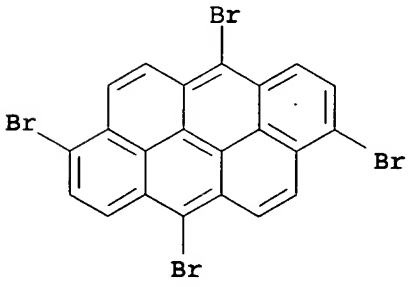
RN 845896-98-2 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED

PAGE 1-A



PAGE 2-A

IT **845896-96-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
RN 845896-96-0 HCAPLUS
CN INDEX NAME NOT YET ASSIGNED



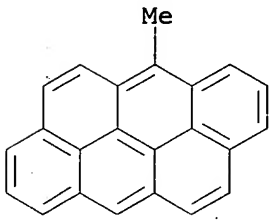
IC ICM H05B033-14
ICS C09K011-06
NCL 428690000; 428917000; 313504000; 313506000; 252301160
CC 73-11 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)
Section cross-reference(s): 74
ST phosphor perylene anthanthrene **electroluminescent** display
IT **Electroluminescent** devices
(displays; fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
IT Luminescent screens
(**electroluminescent**; fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
IT Phosphors
(fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
IT 845896-91-5P 845896-93-7P **845896-94-8P**
845896-97-1P 845896-98-2P 845896-99-3P
845897-00-9P
RL: DEV (Device component use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
IT 90-30-2, N-Phenyl-1-naphthylamine 101-70-2, 4,4'-Dimethoxydiphenylamine 620-93-9, Di-p-tolylamine 1205-64-7, 3-Methyldiphenylamine 56752-35-3, 3.,9-Dibromoperylene 85514-20-1, 3,10-Dibromoperylene 154230-29-2 **845896-96-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)
IT 845896-92-6P 845897-01-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(fluorescent material, organic **electroluminescent** element and organic **electroluminescent** display using perylene and anthanthrene derivs.)

L29 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:199197 Document No. 140:374083 Polycyclic Aromatic Hydrocarbons and Olive Pomace Oil. Guillen, Maria D.; Sopelana, Patricia; Palencia, Gemma (Tecnologia de Alimentos, Facultad de Farmacia, Universidad del Pais Vasco, Vitoria, 01006, Spain). Journal of Agricultural and Food Chemistry, 52(7), 2123-2132 (English) 2004. CODEN: JAFCAU. ISSN: 0021-8561. Publisher: American Chemical Society.
AB The occurrence of polycyclic aromatic hydrocarbons (PAHs) in 5 samples of olive pomace oil was studied to determine the contamination degree of this type of oil and to evaluate if specific purification steps must be introduced during its manufacture The PAHs present have been determined by gas chromatog.-mass spectrometry. A high number of PAHs, with a wide range of mol. wts. and in very high concns., were found in 4 of the samples studied. A very high number of alkyl derivs. and, in many cases, in higher concns. than their resp. parent PAHs, were also

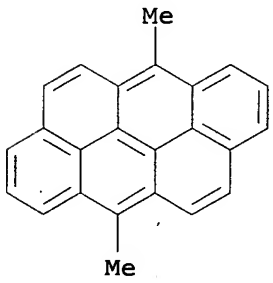
identified. One of the samples, however, presents a more reduced number of PAHs and in significantly lower concns. than the others. These findings reveal that it is necessary to introduce adequate cleanup steps in the manufacturing process of olive pomace oil, which can give rise to oils with a relatively low content of PAHs. Some carcinogenic PAHs were also identified, both unalkylated and alkylated.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)
(polycyclic aromatic hydrocarbons and olive pomace oil)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 17-1 (Food and Feed Chemistry)

IT 50-32-8, Benzopyrene, analysis 53-70-3, Dibenz[a,h]anthracene 56-49-5, 3-Methylcholanthrene 56-55-3, Benz[a]anthracene 57-97-6 83-32-9, Acenaphthene 84-15-1, o-Terphenyl 85-01-8, Phenanthrene, analysis 86-73-7, Fluorene 90-12-0, 1-Methylnaphthalene 91-20-3, Naphthalene, analysis 91-57-6, 2-Methylnaphthalene 92-06-8, m-Terphenyl 92-94-4, p-Terphenyl 120-12-7, Anthracene, analysis 129-00-0, Pyrene, analysis 189-55-9, Dibenzo[a,i]pyrene 189-64-0, Dibenzo[a,h]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Dibenzo[def,mno]chrysene 191-30-0, Dibenzo[a,l]pyrene 192-51-8, Dibenzo[e,l]pyrene 192-65-4, Dibenzo[a,e]pyrene 192-97-2, Benzo[e]pyrene 193-39-5, Indeno[1,2,3-cd]pyrene 195-19-7, Benzo[c]phenanthrene 198-55-0, Perylene 203-33-8, Benzo[a]fluoranthene 205-82-3, Benzo[j]fluoranthene 205-99-2, Benzo[b]fluoranthene 206-44-0,

Fluoranthene 208-96-8, Acenaphthylene 213-46-7, Picene 214-17-5, Benzo[b]chrysene 215-58-7, Dibenz[a,c]anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 238-82-4, 1H-Benzo[a]fluorene 316-14-3, 6-Methylbenz[a]anthracene 316-49-4, 4-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 571-58-4, 1,4-Dimethylnaphthalene 571-61-9, 1,5-Dimethylnaphthalene 575-37-1, 1,7-Dimethylnaphthalene 575-43-9, 1,6-Dimethylnaphthalene 581-40-8, 2,3-Dimethylnaphthalene 581-42-0, 2,6-Dimethylnaphthalene 613-12-7, 2-Methylanthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 781-43-1, 9,10-Dimethylanthracene 832-69-9, 1-Methylphenanthrene 832-71-3, 3-Methylphenanthrene 883-20-5, 9-Methylphenanthrene 1321-94-4, Methylnaphthalene 1523-23-5, 5,10-Dimethylanthracene 1705-85-7, 6-Methylchrysene 1706-01-0 2319-96-2, 5-Methylbenz[a]anthracene 2381-15-9, 10-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2531-84-2, 2-Methylphenanthrene 2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3351-30-2, 4-Methylchrysene 3351-31-3, 3-Methylchrysene 3351-32-4, 2-Methylchrysene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-27-6, 5,6-Dimethylchrysene 3697-30-1, 7-Ethylbenz[a]anthracene 4076-39-5, 1-Methylbenzo[c]phenanthrene 4076-40-8, 4-Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene 5385-75-1, Dibenzo[a,e]fluoranthene 6111-78-0, 11-Methylbenz[a]anthracene 14250-05-6, 5,12-Dimethylchrysene 14458-76-5, 1H-Benzo[b]fluorene 16301-03-4, 7,12-Dimethylbenzo[b]chrysene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene 16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 19557-82-5, 1H-Benzo[c]fluorene 20627-31-0 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene 21297-22-3, 5,12-Dimethylbenz[a]anthracene 22349-59-3, 1,4-Dimethylphenanthrene 25889-60-5, 1-Methylfluoranthene 27138-19-8, Ethylnaphthalene 27208-37-3, Cyclopenta[cd]pyrene 28804-88-8, Dimethylnaphthalene 29062-98-4, Dimethylphenanthrene 31647-36-6, 5-Methylbenzo[a]pyrene 31711-53-2, Methylphenanthrene **31927-64-7**, 6-Methylanthanthrene 33543-31-6, 2-Methylfluoranthene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 41637-90-5, Methylchrysene 56832-73-6, Benzofluoranthene 58429-99-5, 9,10-Dimethylbenz[a]anthracene 58615-36-4, Dibenzopyrene 63019-22-7, 2,3-Dimethylchrysene 63041-61-2, 1,3-Dimethylcholanthrene 63041-62-3, 2,3-Dimethylcholanthrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene 65357-69-9, Methylbenzopyrene 78694-66-3, 6-Ethylbenzo[a]pyrene RL: ANT (Analyte); POL (Pollutant); ANST (Analytical study); OCCU (Occurrence)

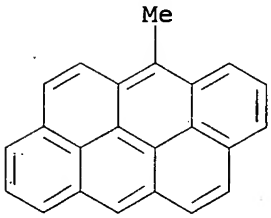
(polycyclic aromatic hydrocarbons and olive pomace oil)

L29 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
1994:648383 Document No. 121:248383 Predicting Carcinogenicity of Polycyclic Aromatic Hydrocarbons from Back-Propagation Neural Network. Villemin, Didier; Cherqaoui, Driss; Mesbah, Abdelhalim (Ecole Nationale Superieure d'Ingenieurs de Caen, I.S.M.R.A., Caen, 14050, Fr.). Journal of Chemical Information and Computer Sciences, 34(6), 1288-93 (English) 1994. CODEN: JCISD8. ISSN: 0095-2338.

AB Models of relationships between structure and carcinogenicity of polycyclic aromatic hydrocarbons were constructed by means of a multilayer neural network using the back-propagation algorithm. The mol. descriptors used were derived from graph theory. The neural network (NN) was used to classify the compds. studied into two categories, namely inactive or active. To evaluate the predictive power of an NN model, the cross-validation procedure was used. The total prediction accuracy of 86% (90% of the actives correctly identified) provided an evidence of the usefulness of the present neural algorithm.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenicity of, back-propagation neural network for prediction of)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



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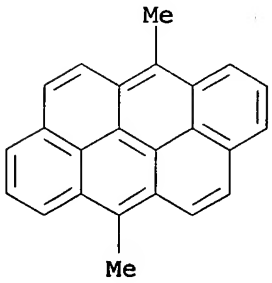


CC 4-6 (Toxicology)
IT 50-32-8, Benzo[a]pyrene, biological studies 53-70-3, Dibenz[a,h]anthracene 56-55-3, Benzo[a]anthracene 57-97-6,

7,12-DiMethylbenz[a]anthracene 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 92-24-0, Naphthacene 120-12-7, Anthracene, biological studies 129-00-0, Pyrene, biological studies 135-48-8, Pentacene 188-52-3, Dibenzo[c,g]phenanthrene 189-55-9, Dibenzo[a,i]pyrene 189-64-0, Dibenzo[a,h]pyrene 191-07-1, Coronene 191-24-2, Benzo[g,h,i]perylene 191-30-0, Dibenzo[a,l]pyrene 192-47-2, Tribenzo[a,e,i]pyrene 192-51-8, Dibenzo[e,l]pyrene 192-65-4, Dibenzo[a,e]pyrene 192-97-2, Benzo[e]pyrene 194-69-4, Benzo[c]chrysene 195-00-6, Anthra[1,2-a]anthracene 195-06-2, Dibenzo[b,g]phenanthrene 195-19-7, Benzo[c]phenanthrene 196-42-9, Naphtho[2,3-a]pyrene 196-78-1, Benzo[g]chrysene 198-55-0, Perylene 213-46-7, Picene 214-17-5, Benzo[b]chrysene 215-26-9, Naphtho[1,2-b]triphenylene 215-58-7, Dibenz[a,c]anthracene 217-54-9, Dibenzo[b,k]chrysene 217-59-4, Triphenylene 218-01-9, Chrysene 222-54-8, Benzo[c]pentaphene 222-93-5, Pentaphene 224-41-9, Dibenz[a,j]anthracene 226-86-8, Dibenzo[a,l]naphthacene 226-88-0, Benzo[a]naphthacene 227-04-3, Dibenzo[a,j]naphthacene 313-74-6, 1,12-DiMethylbenz[a]anthracene 316-14-3, 6-Methylbenz[a]anthracene 316-49-4, 4-Methylbenz[a]anthracene 317-64-6, 6,8-DiMethylbenz[a]anthracene 568-81-0, 6,12-DiMethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 781-43-1, 9,10-Dimethylanthracene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-15-9, 10-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3351-28-8, 1-Methylchrysene 3351-30-2, 4-Methylchrysene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5 4076-40-8, 4-Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene 16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3, 6,8,12-TriMethylbenz[a]anthracene 31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 54986-63-9 63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenicity of, back-propagation neural network for prediction of)

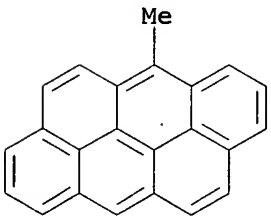
L29 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN
1992:250193 Document No. 116:250193 Correlation studies of anodic peak potentials and ionization potentials for polycyclic aromatic

hydrocarbons. Cremonesi, Paolo; Rogan, Eleanor; Cavalieri, Ercole (Med. Cent., Univ. Nebraska, Omaha, NE, 68198-6805, USA). Chemical Research in Toxicology, 5(3), 346-55 (English) 1992. CODEN: CRTOEC. ISSN: 0893-228X.

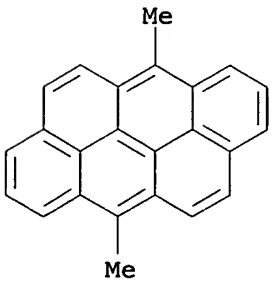
AB The principal aim of this study was to provide a general and simple technique suitable for obtaining ionization potential (IP) of polycyclic aromatic hydrocarbons (PAH) with satisfactory accuracy. Anodic peak potentials (Eap) of 90 PAH were measured by cyclic voltammetry under irreversible oxidation conditions and correlated with the corresponding IP. This allowed determination of a least-squares regression line. From the corresponding equation, IP = 1.70Eap + 5.29, IP can be calculated with a narrow margin of error after a simple electrochem. measure. It was also found that PAH substituted with a Me group on a position of appreciable electron d. are best represented by a different line, corresponding to the equation IP = 1.65Eap + 5.27. The calculated IP were also compared to other tabulated values, determined by different exptl. techniques, and this set of IP values proved to yield the most satisfactory correlation. For some PAH, further studies under reversible voltammetric conditions allowed determination of two addnl. parameters: formal oxidation potentials (E°) and the number of electrons (n) involved in the redox process. IP is an important parameter in predicting the metabolic activation of carcinogenic PAH.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(ionization potential of, carcinogenicity in relation to)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT 50-32-8, Benzo[a]pyrene, biological studies 53-70-3, Dibenz[a,h]anthracene 56-49-5, 3-Methylcholanthrene 56-55-3, Benz[a]anthracene 57-97-6 91-20-3, Naphthalene, biological studies 92-24-0, Naphthacene 120-12-7, Anthracene, biological studies 129-00-0, Pyrene, biological studies 189-55-9, Benzo[rst]pentaphene 189-64-0, Dibenzo[b,def]chrysene 189-92-4, 10-Azabenzo[a]pyrene 191-24-2, Benzo[ghi]perylene 191-26-4, Anthanthrene 191-30-0, Dibenzo[a,l]pyrene 192-47-2, Tribenzo[a,e,i]pyrene 192-51-8, Dibenzo[e,l]pyrene 192-65-4, Naphtho[1,2,3,4-def]chrysene 192-97-2, Benzo[e]pyrene 195-19-7, Benzo[c]phenanthrene 198-55-0, Perylene 213-46-7, Picene 215-58-7, Dibenz[a,c]anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 224-41-9, Dibenz[a,j]anthracene 316-14-3, 6-Methylbenz[a]anthracene 316-49-4, 4-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 737-22-4 781-43-1, 9,10-Dimethylanthracene 794-00-3 2319-96-2, 5-Methylbenz[a]anthracene 2381-15-9, 10-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2541-69-7 3351-28-8, 1-Methylchrysene 3351-30-2, 4-Methylchrysene 3351-31-3, 3-Methylchrysene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4514-19-6, 12-Methylbenzo[a]pyrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 17750-93-5, 7,8,9,10-Tetrahydrobenzo[a]pyrene 18868-66-1 20627-34-3 21248-00-0 21248-01-1, 6-Chlorobenzo[a]pyrene 25732-74-5, 3,4-Dihydrocyclopenta[cd]pyrene 27208-37-3, Cyclopenta[cd]pyrene 31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 53555-67-2, 6-Acetoxybenzo[a]pyrene 59417-86-6, 6-Fluorobenzo[a]pyrene 61735-77-1 61735-78-2 63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene 67242-54-0 68141-56-0 70644-19-8, 9-Methylbenzo[a]pyrene 71171-92-1, 8-Fluorobenzo[a]pyrene 71171-93-2, 9-Fluorobenzo[a]pyrene 71172-11-7 71172-13-9 71511-38-1, 7-Fluorobenzo[a]pyrene 73368-38-4 74018-58-9, 10-Fluorobenzo[a]pyrene 74924-89-3, 8-Fluoro-3-methylcholanthrene 74924-90-6 78694-66-3
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(ionization potential of, carcinogenicity in relation to)

=> => d l32 1-7 cbib abs hitstr hitind

L32 ANSWER 1 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:62881 Document No. 86:62881 Effect of the nearness of electronic levels in di- and tetrahydroxy derivatives of anthraquinone on the deactivation of excited states. Shcheglova, N. A.; Shigorin, D. N.; Dokunikhin, N. S. (Vses. Nauchno-Issled. Fiz.-Khim. Inst. im.

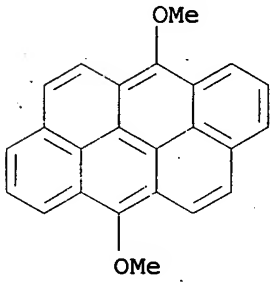
Karpova, Moscow, USSR). Zhurnal Fizicheskoi Khimii, 50(9), 2320-4 (Russian) 1976. CODEN: ZFKHA9. ISSN: 0044-4537.

AB The effect of the nearness of electronic levels on the deactivation process of excited states is discussed in the case of di- and tetrahydroxyanthraquinones characterized by various degrees of nearness of Snπ*, S2pzπ* and Tnπ* electronic levels. As a parameter characterizing the process of radiationless deactivation, the quantum yield of **luminescence** was studied. α-Hydroxyanthraquinones were characterized by different quantum yields. It reflected different degrees of nearness of the electronic levels, which indicated various deactivation mechanisms of excited states of the compds. Changes in conformation of the systems occurring in conversion of ground states to excited one influenced the value of the quantum yield.

IT **57981-28-9**
RL: PROC (Process)
(**luminecence** quenching of)

RN 57981-28-9 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6,12-dimethoxy- (9CI) (CA INDEX NAME)



CC 73-3 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
Section cross-reference(s): 74, 72

ST anthraquinone hydroxy excited state deactivation; energy level hydroxyanthraquinone; radiationless deactivation hydroxyanthraquinone; **luminescence** hydroxyanthraquinone

IT **Luminescence** quenching
(of dimethoxyanthracene and dimethoxyanthanthrene)

IT **Luminescence**
(of hydroxyanthraquinones, quantum yield in relation to radiationless deactivation of)

IT 2395-97-3 **57981-28-9**
RL: PROC (Process)
(**luminecence** quenching of)

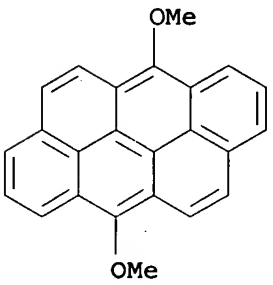
L32 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN

1976:42753 Document No. 84:42753 Effect of the symmetry of molecules on some of their spectral characteristics. Shcheglova, N. A.; Rogovin, V. I. (Nauchno-Issled. Fiz. Khim. Inst. im. Karpova, Moscow, USSR). Zhurnal Fizicheskoi Khimii, 49(10), 2546-51 (Russian) 1975. CODEN: ZFKHA9. ISSN: 0044-4537.

GI For diagram(s), see printed CA Issue.

AB The absorption and **luminescence** spectra of I and II at 77 and 298°K were given and compared with the spectra of III. The decreased internal conversion on lowering the temperature was related to the lower probability and amplitude of twisting and bending vibrations.

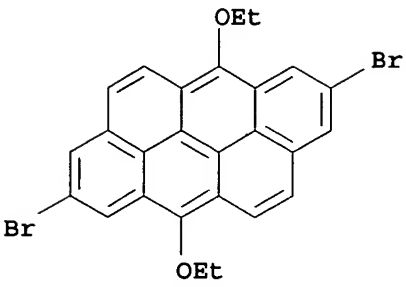
IT **57981-28-9**
RL: PRP (Properties)
(absorption and **luminescence** spectra of)
RN 57981-28-9 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethoxy- (9CI) (CA INDEX NAME)



CC 22-2 (Physical Organic Chemistry)
ST spectra dimethoxyanthracene dimethoxyanthanthrene; **luminescence** dimethoxyanthracene dimethoxyanthanthrene; anthracene dimethoxy spectra **luminescence**; anthanthrene dimethoxy spectra **luminescence**
IT **Luminescence**
Ultraviolet and visible spectra
(of dimethoxyanthracene and -anthanthrene)
IT 2395-97-3 6119-74-0 **57981-28-9**
RL: PRP (Properties)
(absorption and **luminescence** spectra of)

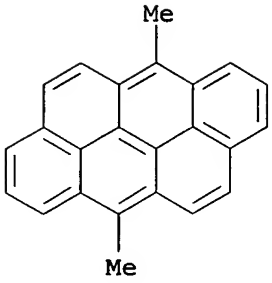
L32 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
1973:459998 Document No. 79:59998 Photodesensitizable thermographic copy sheets. Burleigh, Malcolm B. (Minnesota Mining and Manufacturing Co.). Ger. Offen. DE 2245234 19730322, 43 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1972-2245234 19720912.
GI For diagram(s), see printed CA Issue.
AB Materials less sensitive to high temps. and humidity and with greater exposure tolerance than those of U.S. 3,094,417 (Belg. 612,241; CA 57: 16042a) have 2.5-13 μ layers of a binder containing 0.05-2% of a dye with ≥2 units of 3 fused benzene rings with a total of 2 solubilizing ether and 2-4 auxochromic (Br, Cl) groups. Suitable dyes **fluoresce** in 0.001 M solution when irradiated at 200-400 nm. They activate O when exposed at 400-700 nm and thus deactivate an acceptor such as a 1-naphthol, hydrazone, or dithiooxamide of which the layer contains 1-8%. When contacted with a receptor sheet (U.S. 3,218,166; Belg. 640,183; CA 63: 3813e) containing a metal soap, such as Ag behenate, at 90-150° the salt is reduced by the unaffected naphthol. Thus, I, a typical dye, was obtained from Vat Violet 1 by reduction with alkaline Na2S2O4 and treatment with Et2SO4. A 25 μ Mylar film was coated with a solution of 0.02 part dye in 2 parts CHCl3, mixed with BuOH 8 parts and Me2CO 87 parts, then with Ethocel 5 parts and 4-methoxy-1-naphthol 0.2 part. From the exposed sheet a copy was obtained by 4-5 sec contact with a receptor sheet between rollers or plates of 125-140°.
IT **42803-67-8**
RL: USES (Uses)
(photodesensitizable copy sheets containing)
RN 42803-67-8 HCAPLUS
CN Dibenzo[def,mno]chrysene, 2,8-dibromo-6,12-diethoxy- (9CI) (CA

INDEX NAME)



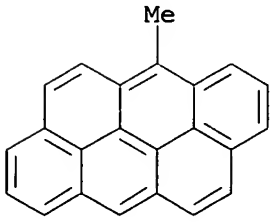
IC G03C
CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT 84-85-5 846-63-9 2216-75-3 16435-04-4 40537-72-2
42803-65-6 42803-66-7 **42803-67-8** 42803-68-9
50354-93-3 50813-25-7
RL: USES (Uses)
(photodesensitizable copy sheets containing)

L32 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
1973:158644 Document No. 78:158644 Oxygen quenching of aromatic triplet states in solution. 1. Gijzeman, O. L. J.; Kaufman, F.; Porter, G. (Davy Faraday Res. Lab., R. Inst., London, UK). Journal of the Chemical Society, Faraday Transactions 2: Molecular and Chemical Physics, 69(Pt. 5), 708-20 (English) 1973. CODEN: JCFTBS. ISSN: 0300-9238.
AB Rate consts. for the O quenching of aromatic hydrocarbon triplets were determined by the laser flash photolysis technique. The quenching of high triplet energy compds. was characterized by rates which were inversely proportional to triplet energy. The reaction probabilities, which were as small as 10-2 in hexane, increased in polar or viscous solvents. Mols. with low triplet energies were quenched at one-ninth the measured diffusion controlled encounter rate. The results were explained by nonradiative transitions of a collision complex of aromatic triplet and ground state O. The data were consistent with electronic matrix elements for the energy transfer quenching processes that are dependent on orbital symmetry matching and charge transfer interactions. The importance of restrictive Franck-Condon factors were discussed.
IT **41217-05-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)

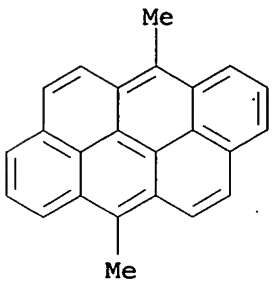


CC 22-4 (Physical Organic Chemistry)
IT **Fluorescence** quenching
(of aromatic triplet states, by oxygen, solvent effect on)
IT **41217-05-4P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L32 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
1963:426070 Document No. 59:26070 Original Reference No. 59:4695a-b
First triplet of polycyclic aromatic hydrocarbons. I. **Phosphorescent** spectra in the red and the near infrared of solutions congealed at -180°. II. First triplet and cancerigenic activity. Mue, B.; Hubert-Habar, M. (Inst. Radium, Paris). Proc. Intern. Meeting Mol. Spectry., 4th, Bologna, 1959, 2, 647-56, discussion 647 (French) 1962.
AB **Phosphorescent** spectra of benzo-3,4-pyrene (I) and 2 Me derivs., dibenzo-3,4,8,9-pyrene (II) and 2 Me derivs., dibenzo-3,4,9,10-pyrene (III) and 2 Me derivs., anthanthrene (IV) and 2 Me derivs., and perylene (V) were measured at -180°. Toluene was the solvent for all compds. except I, for which 95% EtOH was used. All solns. had a concentration of approx. 100 γ/ml. The height of bands owing to transitions of the 1st triplet to the fundamental state decreased with frequency. Values of the energy of transition from the 1st triplet to the fundamental state, calculated from the band of greatest frequency, were 10% greater than theoretical values for I, II, III, and IV. No **phosphorescence** of pure V was seen. No correlation was found between the height of the 1st triplet and cancerigenic activity.
IT **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl-
41217-05-4, Dibenzo[def,mno]chrysene, 6,12-dimethyl-
(energy levels and **phosphorescence** of, carcinogenicity in relation to)
RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



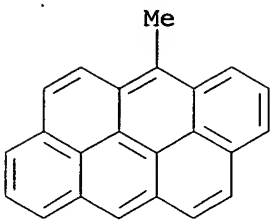
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



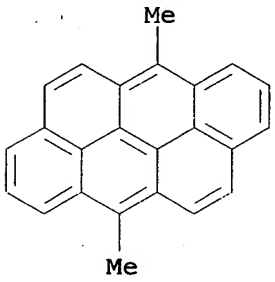
CC 10 (Spectra and Some Other Optical Properties)
IT Carcinogenic substances
(energy levels and **phosphorescence** of)
IT **Phosphorescence**
(of hydrocarbons (aromatic polycyclic), carcinogenicity and)
IT 50-32-8, Benzo[a]pyrene 189-55-9, Benzo[rst]pentaphene 189-64-0, Dibenzo[b,def]chrysene 191-26-4, Dibenzo[def,mno]chrysene 198-55-0, Perylene 5174-22-1, Dibenzo[b,def]chrysene, 7-methyl- **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl- 33942-88-0, Benzo[rst]pentaphene, 5-methyl- **41217-05-4**, Dibenzo[def,mno]chrysene, 6,12-dimethyl- 56309-78-5, Benzo[rst]pentaphene, 5,8-dimethyl- 83439-54-7, Dibenzo[b,def]chrysene, 7,14-dimethyl-
(energy levels and **phosphorescence** of, carcinogenicity in relation to)

L32 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
1961:21094 Document No. 55:21094 Original Reference No. 55:4147e-g
Fluorescence spectra of aromatic hydrocarbons and heterocyclic aromatic compounds. Van Duuren, Benjamin L. (New York Univ., New York). Anal. Chem., 32, 1436-42 (Unavailable) 1960. CODEN: ANCHAM. ISSN: 0003-2700.
AB Spectra are tabulated for indole, carbazole, 5H-benzo[b]carbazole, 7H-dibenzo[a,g]carbazole, 7H-dibenzo[c,g]carbazole, indene, fluorene, 11H-benzo[b]fluorene, benzofuran, dibenzofuran, benzo[b]naphtho[2,3-d]-furan, quinoline, acridene, phenanthridene, dibenz[a,h]-acridene, dibenz[a,j]acridene, naphthacene, benz[a]anthracene, chrysene, triphenylene, picene, acenaphthene, 1,1'-binaphthyl, 2,2'-binaphthyl, 2-phenylnaphthalene, pyrene, benzo[a]pyrene, benzo[e]pyrene, dibenzo[a,l]pyrene, dibenzo[a,i]pyrene, dibenzo[a,h]pyrene, dibenzo[cd,jk]pyrene, dibenzo [de,ke]anthracene, benzo[g,h,i] perylene, dibenzo[ghi,pqr]perylene, 11H-naphtho[2,1-α]fluorene, 13H-naphtho[2,3-b]fluorene, and fluoranthene. Effects on **fluorescence** spectra of replacement of H atoms by alkyl groups, replacement of C by N or O, varying solvent, and concentration are discussed.
IT **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl- **41217-05-4**, Dibenzo[def,mno]chrysene, 6,12-dimethyl-
(**fluorescence** of)
RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX

NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 3 (Electronic Phenomena and Spectra)
IT Heterocyclic compounds
Hydrocarbons
(**fluorescence** of aromatic)
IT **Fluorescence**
(of aromatic hydrocarbons and heterocyclic aromatic compds.)
IT 604-53-5, 1,1'-Binaphthyl
(**fluorescence**)
IT 50-32-8, Benzo[a]pyrene 53-70-3, Dibenz[a,h]anthracene 56-49-5, Cholanthrene, 3-methyl- 56-55-3, Benz[a]anthracene 57-97-6, Benz[a]anthracene, 7,12-dimethyl- 83-32-9, Acenaphthene 85-01-8, Phenanthrene 86-73-7, Fluorene 86-74-8, Carbazole 91-22-5, Quinoline 92-24-0, Naphthacene 95-13-6, Indene 120-12-7, Anthracene 120-72-9, Indole 129-00-0, Pyrene 132-64-9, Dibenzofuran 189-55-9, Benzo[rst]pentaphene 189-64-0, Dibenzo[b,def]chrysene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Dibenzo[def,mno]chrysene 191-30-0, Dibenzo[def,p]chrysene 192-97-2, Benzo[e]pyrene 194-59-2, 7H-Dibenzo[c,g]carbazole 198-55-0, Perylene 203-12-3, Benzo[ghi]fluoranthene 206-44-0, Fluoranthene 207-08-9, Benzo[k]fluoranthene 207-84-1, 7H-Dibenzo[a,g]carbazole 213-46-7, Picene 217-59-4, Triphenylene 218-01-9, Chrysene 220-97-3, 11H-Indeno[2,1-a]phenanthrene 224-41-9, Dibenz[a,j]anthracene 224-42-0, Dibenz[a,j]acridine 226-36-8, Dibenz[a,h]acridine 243-17-4, 11H-Benzo[b]fluorene 243-28-7, 5H-Benzo[b]carbazole 243-42-5, Benzo[b]naphtho[2,3-d]furan 248-93-1, 13H-Indeno[1,2-b]anthracene 260-94-6, Acridine 271-89-6, Benzofuran 316-14-3, Benz[a]anthracene, 6-methyl- 612-78-2, 2,2'-Binaphthyl 612-94-2, Naphthalene, 2-phenyl- 2381-15-9, Benz[a]anthracene, 10-methyl- 2381-16-0,

Benz[a]anthracene, 9-methyl- 2381-31-9, Benz[a]anthracene, 8-methyl- 2422-79-9, Benz[a]anthracene, 12-methyl- 2498-75-1, Benz[a]anthracene, 3-methyl- 2498-76-2, Benz[a]anthracene, 2-methyl- 2498-77-3, Benz[a]anthracene, 1-methyl- 2541-69-7, Benz[a]anthracene, 7-methyl- 3442-78-2, Pyrene, 2-methyl- 6111-78-0, Benz[a]anthracene, 11-methyl- 23339-05-1, Fluoranthene, 7-methyl- 25889-63-8, Fluoranthene, 8,9-dimethyl- **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl- 33543-31-6, Fluoranthene, 2-methyl- **41217-05-4**, Dibenzo[def,mno]chrysene, 6,12-dimethyl- 63041-27-0, Fluoranthene, 1,2,3-trimethyl-
(**fluorescence** of)

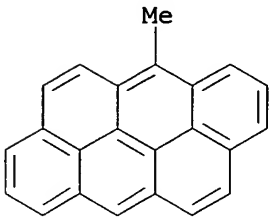
L32 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2005 ACS on STN
1957:99020 Document No. 51:99020 Original Reference No. 51:17866b-g
Polycyclic aromatic hydrocarbons. III. Substitution derivatives of anthanthrene. Buu-Hoi, Ng. Ph.; Lavit, Denise (Univ. Paris). Recueil des Travaux Chimiques des Pays-Bas et de la Belgique, 76, 200-4 (French) 1957. CODEN: RTCPB4. ISSN: 0370-7539.

AB cf. C.A. 51, 4340g, 15480a. Since carcinogenic activity is augmented by meso-substitution in anthracene hydrocarbons, the chemical reactivity of anthanthrene (I) was investigated. Anthanthrone (II) (30 g.), 30 g. powdered Zn, 30 g. NaCl, 150 g. anhydrous $ZnCl_2$ intimately mixed and treated with 5 ml. H_2O, stirred to a paste at 210°, kept several min. at 290°, the cold mass treated with dilute HCl, kept overnight, filtered, and the powdered product dried and crystallized from 1500 ml. anhydrous PhMe containing a trace of hydroquinone yielded 18 g. I, m. 265° (sublimation), deep brown halochromy with H_2SO_4. I (8 g.), 4.7 g. HCON-MePh, and 5.4 g. $POCl_3$ heated 4 hrs. on a steam bath with 8 ml. o-ClC_6H_4Cl, the mixture poured into concentrated aqueous NaOAc, stirred with 50 ml. o-ClC_6H_4Cl, steam-distilled, cooled, filtered, and the product washed with H_2O, dried, and repeatedly crystallized from PhCl gave 4.7 g. 6-anthanthroic aldehyde (III), m. 260°, dark green halochromy in H_2SO_4, vivid green **fluorescence** in hydrocarbon solns.; thiosemicarbazone, m. 275°. III (7.6 g.) in 700 ml. $(CH_2OH)_2$ boiled 2 hrs. with 8 g. 95% N_2H_4. H_2O, treated with 8 g. KOH, boiled 45 min. (loss of H_2O), the cold residue diluted with H_2O, filtered, and the precipitate dried in vacuo and recrystd. from C_6H_6 yielded 5.3 g. 6-methylanthanthrene (IV), m. 192°, deep brown halochromy with H_2SO_4, vivid blue **fluorescence** in C_6H_6, converted by boiling with CrO_3 in AcOH to II, m. 340°, green coloration in H_2SO_4. Formylation of 6.2 g. IV as above gave 3.5 g. 12-formyl-6-methylanthanthrene, m. 328°, green halochromy in H_2SO_4, green **fluorescence** in PhCl, reduced as above to 6,12-dimethylanthanthrene (V), m. 281°, brown-black halochromy and intense blue-green coloration in C_6H_6, oxidized by CrO_3 in AcOH to II. I (0.3 g.) in 75 ml. o-ClC_6H_4Cl treated dropwise with 0.33 g. SO_2Cl_2 in 10 ml. o-ClC_6H_4Cl, the mixture kept at room temperature 24 hrs., filtered, and the washed and dried precipitate recrystd. repeatedly from PhCl yielded 0.1 g. 6,12-dichloroanthanthrene, m. 374°, pale violet-brown halochromy, oxidized to II. Attempts to nitrate I in $PhNO_2$ with HNO_3 (d. 1.52) at room temperature 2 days failed to give any definite nitration product. IV and V are under examination for carcinogenic properties.

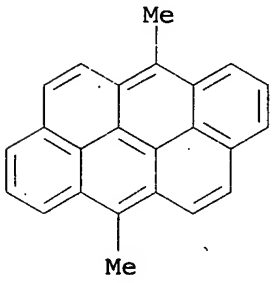
IT **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl-
41217-05-4, Dibenzo[def,mno]chrysene, 6,12-dimethyl-
63040-55-1, Dibenzo[def,mno]chrysene-6-carboxaldehyde
63040-58-4, Dibenzo[def,mno]chrysene-6-carboxaldehyde, 12-methyl- **102442-55-7**, Dibenzo[def,mno]chrysene,

6,12-dichloro- 120233-61-6, Dibenzo[def,mno]chrysene-6-carboxaldehyde, thiosemicarbazone
(preparation of)

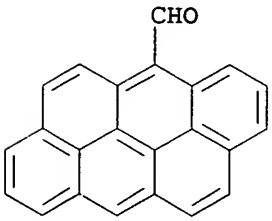
RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



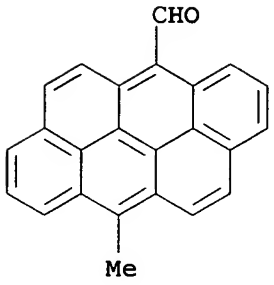
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



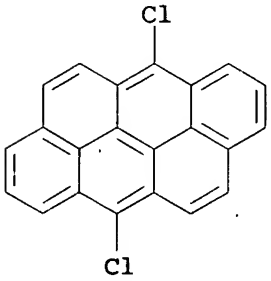
RN 63040-55-1 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-carboxaldehyde (6CI, 7CI, 9CI) (CA INDEX NAME)



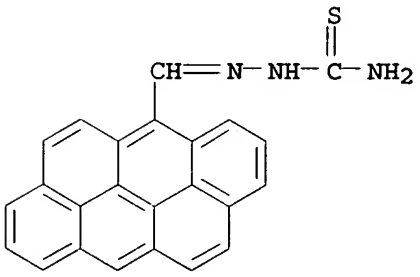
RN 63040-58-4 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-carboxaldehyde, 12-methyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



RN 102442-55-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dichloro- (6CI) (CA INDEX NAME)



RN 120233-61-6 HCAPLUS
CN Dibenzo[cd,jk]pyrene-6-carboxaldehyde, thiosemicarbazone (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)
IT **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl-
41217-05-4, Dibenzo[def,mno]chrysene, 6,12-dimethyl-
63040-55-1, Dibenzo[def,mno]chrysene-6-carboxaldehyde
63040-58-4, Dibenzo[def,mno]chrysene-6-carboxaldehyde, 12-methyl- **102442-55-7**, Dibenzo[def,mno]chrysene, 6,12-dichloro- **120233-61-6**, Dibenzo[def,mno]chrysene-6-carboxaldehyde, thiosemicarbazone
(preparation of)

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L33 ANSWER 1 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

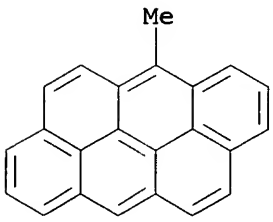
2004:572236 Document No. 141:290173 Fuzzy principal component analysis and its applications in QSAR studies. Sarbu, Costel; Demertzis, Mavroudis A.; Kovala-Demertzi, Dimitra (Fac. Chem. Chem. Eng., "Babes-Bolyai" Univ., Cluj-Napoca, 400028, Rom.). Revista de Chimie (Bucharest, Romania), 55(5), 297-301 (English) 2004. CODEN: RCBUAU. ISSN: 0034-7752. Publisher: SYSCOM 18 SRL.

AB Principal component anal. (PCA) is a favorite tool in anal. chemical and other tech. fields for data compression and information extraction PCA finds linear combinations of the original measurement variables that describe the significant variations in the data. However, it is well-known that PCA, as any other multivariate statistical method, is sensitive to outliers, missing data, and poor linear correlation between variables due to poorly distributed variables. As a result data transformations have a large impact upon PCA. In this regard, one of the most powerful approaches to improve PCA appears to be the fuzzification of the matrix data, thus diminishing the influence of the outliers. In this paper it is discussed and applied a robust fuzzy PCA algorithm (FPCA). The efficiency of the new algorithm is illustrated on a data set concerning the carcinogenic activity of polycyclic aromatic hydrocarbons (PAHs): the first principal component explains 87.25% of the total variance as compared to only 59.95 for PCA. Even more, PCA showed only a partial separation of scores (PAHs) onto the plane described by the first two principal components, whereas a much sharper differentiation of the PAHs, from carcinogenic point of view, is observed when FPCA is applied.

IT **31927-64-7 41217-05-4**
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(fuzzy principal component anal. and its applications in QSAR studies)

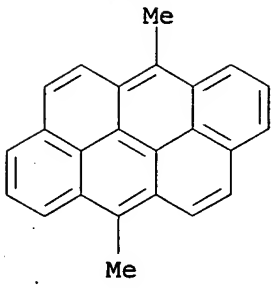
RN 31927-64-7 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-1 (Toxicology)
IT 50-32-8, Benzo[a]pyrene, biological studies 53-70-3, Dibenz[a,h]anthracene 56-55-3, Benz[a]anthracene 57-97-6 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[c,g]phenanthrene 189-55-9, Benzo[rst]pentaphene 189-64-0, Dibenzo[b,def]chrysene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Dibenzo[def,mno]chrysene 191-30-0, Dibenzo[def,p]chrysene 192-47-2, Dibenzo[h,rst]pentaphene 192-51-8, Dibenzo[fg,op]naphthacene 192-65-4, Naphtho[1,2,3,4-def]chrysene 192-97-2, Benzo[e]pyrene 194-69-4, Benzo[c]chrysene 195-19-7, Benzo[c]phenanthrene 196-42-9, Naphtho[2,1,8-qra]naphthacene 196-78-1, Benzo[g]chrysene 213-46-7, Picene 215-26-9, Naphtho[1,2-b]triphenylene 215-58-7, Benzo[b]triphenylene 217-59-4, Triphenylene 218-01-9, Chrysene 222-54-8, Benzo[c]pentaphene 224-41-9, Dibenz[a,j]anthracene 226-88-0, Benzo[a]naphthacene 239-98-5, Benzo[a]pentacene 316-14-3 317-64-6 568-81-0 652-04-0 1705-85-7 2319-96-2 2381-16-0 2381-19-3 2381-21-7 2381-31-9 2381-34-2 2381-39-7 2422-79-9 2498-75-1 2498-76-2 2498-77-3 2541-69-7 2606-85-1 3353-12-6 3442-78-2 3697-24-3 4076-39-5 4076-40-8 4514-19-6 6111-78-0 16757-80-5 16757-81-6 16757-82-7 16757-83-8 16757-84-9 16757-85-0 16757-86-1 16757-87-2 16757-88-3 16757-89-4 16757-90-7 16757-91-8 20627-34-3 31647-36-6 **31927-64-7** 40568-90-9 **41217-05-4** 60032-75-9, Tribenzo[b,def,p]chrysene 63041-76-9 63041-77-0 63104-32-5 63104-33-6 70644-19-8 82721-25-3
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(fuzzy principal component anal. and its applications in QSAR studies)

L33 ANSWER 2 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2004:41551 Document No. 140:112197 Nucleation inhibitor, crystalline resin composition and method of controlling crystallization of crystalline resin composition. Takeuchi, Hiroshi; Sukata, Kazuaki (Orient Chemical Industries, Ltd., Japan). PCT Int. Appl. WO 2004005389 A1 20040115, 194 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU,

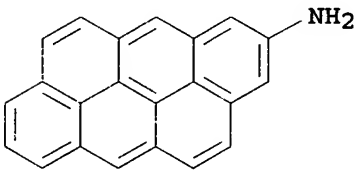
MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2003-JP8580 20030707. PRIORITY: JP 2002-200674 20020709.

AB A nucleation inhibitor comprises a compound being any of compds. having at least one structure selected from among polycyclic structures obtained through condensation cyclization of three or more ≥4-membered cyclic structures, the compds. not including nigrosine, aniline black and copper phthalocyanine derivs. Thus, 100 parts refined polyamide 66 (Zytel 101L) and 10 parts 1-aminoanthracene (I)were added to 2,2,2-trifluoroethanol, heat dissolved, left still, stripped of the solvent, and dried in vacuo to give test pieces, showing crystallization temperature 218.5°, compared with 232.8° without I.

IT **646060-26-6**, Dibenzo[def,mno]chrysen-2-amine
RL: MOA (Modifier or additive use); USES (Uses)
(nucleation inhibitor; polycyclic nucleation inhibitor for controlling crystallization of crystalline resin composition)

RN 646060-26-6 HCAPLUS

CN Dibenzo[def,mno]chrysen-2-amine (9CI) (CA INDEX NAME)



IC ICM C08K005-00
ICS C08L101-00

CC 37-6 (Plastics Manufacture and Processing)
Section cross-reference(s): 25

IT 81-30-1 82-45-1 89-32-7 92-35-3 128-64-3 128-95-0 132-32-1 153-78-6, 9H-Fluoren-2-amine 177-88-8 190-26-1, Ovalene 191-07-1, Coronene 191-13-9, Pyranthrene 191-48-0, Diacenaphtho[1,2-j:1',2'-l]fluoranthene 196-62-3, Trinaphthylene 202-85-7 214-16-4, Anthra[2,1-a]naphthacene 214-83-5, Diquinoxalino[2,3-a:2',3'-c]phenazine 222-78-6, Hexaphene 258-38-8, Heptacene 298-81-7 434-84-4, [9,9'-Bianthracene]-10,10'(9H,9'H)-dione 484-11-7 494-38-2 519-23-3 610-49-1, 1-Aminoanthracene 613-13-8, 2-Anthracenamine 655-86-7, 2,3-Phenazinediamine 716-39-2, Naphtho[2,3-c]furan-1,3-dione 779-26-0 781-73-7 789-47-9, 2-Chrysenamine 1086-80-2 1134-35-6 1207-12-1 1606-67-3, 1-Pyrenamine 1660-93-1 1662-01-7 2222-33-5, 5H-Dibenzo[a,d]cyclohepten-5-one 2381-40-0 2498-66-0, Benz[a]anthracene-7,12-dione 2516-05-4 2550-73-4 2693-46-1, 3-Fluoranthenamine 3133-07-1 3248-05-3 3264-21-9 3366-65-2, 2-Phenanthrenamine 4106-66-5, 3-Dibenzofuranamine 4379-54-8, 1H-Benz[f]isoindole-1,3(2H)-dione 4523-48-2, 4-Acenaphthylenamine 4657-97-0 4733-39-5 4756-92-7 5298-71-5 5651-60-5, Benz[d]indeno[1,2-b]pyran-5,11-dione 5725-89-3 5960-69-0 6050-13-1, Dibenz[c,e]oxepin-5,7-dione 6051-87-2 6272-55-5 6344-63-4, 9H-Fluoren-1-amine 6373-11-1, 1,2-Aceanthrylenedione 6398-59-0 6967-04-0 7385-67-3 7415-79-4 14533-04-1 17169-81-2, 2-Triphenylenamine 18158-43-5 18605-42-0 20061-68-1 20315-68-8 27591-97-5 31301-28-7 33923-98-7 35359-28-5 36378-29-7 52009-64-0 52837-55-5 55011-44-4 55592-69-3 55716-75-1, 2-Biphenylenamine 55804-67-6 62669-74-3 63041-77-0 65558-69-2 67122-24-1 67867-47-4

68151-08-6 69706-40-7, 4H-Cyclopenta[def]phenanthren-2-amine
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Benzo[a]pyren-1-amine 95689-92-2 102491-77-0 114459-05-1
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2-Pentacenamine 173471-26-6 173471-54-0, 2-Hexacenamine
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8-Aceanthrylenamine 646058-53-9 646058-54-0,
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646059-51-0 646059-57-6 646059-59-8 646059-60-1 646059-61-2
646059-63-4 646059-64-5 646059-68-9 646059-69-0,
Dicyclopenta[a,f]naphthalen-2-amine 646059-71-4,
Dicyclopenta[b,g]naphthalen-2-amine 646059-77-0,
Benzo[a]naphthacen-3-amine 646059-79-2, Benzo[b]chrysen-2-amine
646059-82-7, Benzo[a]pyren-8-amine 646059-85-0 646059-91-8,
Benzo[b]triphenylen-11-amine 646059-92-9, Dibenz[a,h]anthracen-3-amine 646059-93-0, Benzo[k]fluoranthen-9-amine 646059-95-2,
Benz[e]acephenanthrylen-10-amine 646059-98-5, 3-Picenamine
646060-01-7, 6,7-Pentaphenediamine 646060-04-0 646060-09-5
646060-13-1 646060-19-7, 1H-Benzo[de]pentacen-12-amine
646060-22-2 646060-24-4, Naphtho[2,1,8-qra]naphthacen-2-amine
646060-26-6, Dibenzo[def,mno]chrysen-2-amine 646060-30-2,
Benzo[ghi]perylen-6-amine 646060-33-5, Dibenzo[b,def]chrysen-2-amine 646060-47-1 646060-55-1 646060-58-4,
Anthra[9,1,2-cde]pentaphene 646060-60-8 646060-67-5
646060-69-7 646060-71-1 646060-76-6 646060-79-9 646060-81-3
646060-82-4 646060-84-6 646060-86-8
RL: MOA (Modifier or additive use); USES (Uses)
(nucleation inhibitor; polycyclic nucleation inhibitor for controlling crystallization of crystalline resin composition)

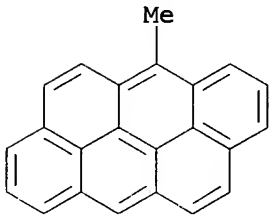
L33 ANSWER 4 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:810953 Document No. 138:34577 Identifying Relevant Molecular Descriptors Related to Carcinogenic Activity of Polycyclic Aromatic Hydrocarbons (PAHs) Using Pattern Recognition Methods. Coluci, V. R.; Vendrame, R.; Braga, R. S.; Galvao, D. S. (Instituto de Fisica, UNICAMP, Campinas, 13083-970, Brazil). Journal of Chemical Information and Computer Sciences, 42(6), 1479-1489 (English) 2002. CODEN: JCISD8. ISSN: 0095-2338. Publisher: American Chemical Society.

AB Polycyclic Aromatic Hydrocarbons (PAHs) constitute an important family of mols. capable of inducing chemical carcinogenesis. In this work we report structure-activity relationship (SAR) studies for 81 PAHs using the pattern-recognition methods Principal Component Anal. (PCA), Hierarchical Clustering Anal. (HCA) and Neural Networks (NN). The used mol. descriptors were obtained from the semiempirical Parametric Method 3 (PM3) calcns. We have developed a new procedure that is capable of identifying the PAHs' carcinogenic activity with an accuracy higher than 80%. PCA selected mol. descriptors that can be directly correlated with some models proposed to PAHs' metabolic activation mechanism leading to the formation of PAHs-DNA adducts.

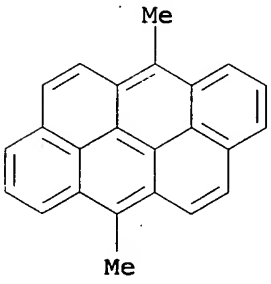
PCA, HCA and NN validate the energy separation between the HOMO and its next lower level as a major descriptor defining the carcinogenic activity. This descriptor has been only recently discussed in the literature as one new possible universal parameter for defining the biol. activity of several classes of compds.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(identifying relevant mol. descriptors related to carcinogenic activity of polycyclic aromatic hydrocarbons using pattern recognition methods)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)

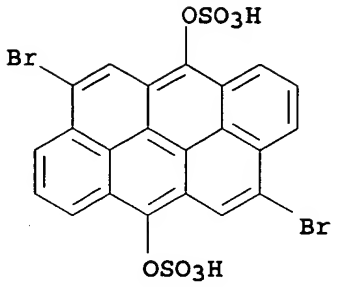


CC 4-6 (Toxicology)

IT 50-32-8, Benzo[3,4]pyrene, biological studies 53-70-3, Dibenzo[1,2;5,6]anthracene 56-55-3, Benz[1,2]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[3,4;5,6]phenanthrene 189-55-9, Dibenzo[3,4;9,10]pyrene 189-64-0, Dibenzo[3,4;8,9]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Anthanthrene 191-30-0, Dibenzo[1,2;3,4]pyrene 192-47-2, Dibenzo[h,rst]pentaphene 192-51-8, Dibenzo[fg,op]naphthacene 192-65-4, Dibenzo[3,4;6,7]pyrene 192-97-2, Benzo[1,2]pyrene 194-69-4, Dibenzo[1,2;5,6]phenanthrene 195-19-7, Benzo[3,4]phenanthrene 196-42-9, Naphtho[2,1,8-qra]naphthacene 196-78-1, Dibenzo[1,2;3,4]phenanthrene 213-46-7, Picene 215-26-9, Naphtho[1,2-b]triphenylene 215-58-7,

Dibenzo[1,2;3,4]anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 222-54-8, Benzo[c]pentaphene 224-41-9, Dibenzo[1,2;7,8]anthracene 226-88-0, Benzo[1,2]naphthacene 239-98-5, Benzo[1,2]pentacene 316-14-3, 6-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5, 1-Methylbenzo[c]phenanthrene 4076-40-8, 4-Methylbenzo[c]phenanthrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene 16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene 31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 60032-75-9, Tribenzo[3,4;6,7;8,9]pyrene 63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene 70644-19-8, 9-Methylbenzo[a]pyrene 82721-25-3, 6,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(identifying relevant mol. descriptors related to carcinogenic activity of polycyclic aromatic hydrocarbons using pattern recognition methods)

L33 ANSWER 5 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:650106 Document No. 137:187166 Full color printing by using ink-jet inks. Sakai, Taizaburo (Japan). Jpn. Kokai Tokkyo Koho JP 2002241661 A2 20020828, 17 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2001-86433 20010216.
AB The inks contain 7 colors composed of cyan (C), magenta (M), yellow (Y), red (R), green (G), blue (B), and black (K). The inks provide beautiful full color images. Thus, an ink-jet ink containing 7 colors of vat dyes was exemplified.
IT **10290-03-6**
RL: TEM (Technical or engineered material use); USES (Uses)
(full color printing by using ink-jet inks of CMYRGBK system)
RN 10290-03-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



●2 Na

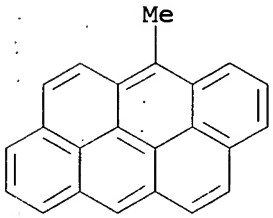
IC ICM C09D011-00
ICS B41J002-21; B41J002-01; B41M005-00
CC 42-12 (Coatings, Inks, and Related Products)
IT 1324-57-8 1324-72-7 2519-28-0 2538-84-3 2702-33-2
2747-19-5 3875-70-5 3875-72-7 3956-62-5 6535-53-1
10126-86-0 10126-87-1 10126-91-7 10134-35-7 **10290-03-6**
13109-68-7 106383-49-7 217189-48-5 217189-49-6 217189-50-9
217189-51-0 443304-10-7 443304-11-8 449728-02-3 449728-03-4
449728-04-5 449742-41-0
RL: TEM (Technical or engineered material use); USES (Uses)
(full color printing by using ink-jet inks of CMYRGBK system)

L33 ANSWER 6 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:584153 Document No. 138:132474 Support vector machine classification of the carcinogenic activity of polycyclic aromatic hydrocarbons. Ivanciuc, Ovidiu (Sealy Center for Structural Biology, Department of Human Biological Chemistry & Genetics, University of Texas Medical Branch, Galveston, TX, 77555-1157, USA). Internet Electronic Journal of Molecular Design [online computer file], 1(4), 203-218 (English) 2002. CODEN: IEJMAT. ISSN: 1538-6414. URL: http://biochempress.com/iejmd_2002_1_0203.pdf Publisher: BioChem Press.
AB Motivation: Structure-activity relationships (SAR) can be efficiently used to predict the carcinogenic hazard of new chems., before producing them on a large scale or even before synthesizing them. SAR models that detect potential carcinogens can also supplement short-term tests of genotoxicity, long-term tests of carcinogenicity in rodents, or epidemiol. evidence in humans. Method: Support vector machine (SVM) is an efficient classification algorithm that can provide highly predictive SAR models for the carcinogenic hazard. The authors have applied the SVM model to identify the carcinogenic activity of 46 methylated and 32 non-methylated polycyclic aromatic hydrocarbons (PAH). The PAH chemical structure was encoded by four theor. descriptors computed with PM3, namely the energy of the HOMO EHOMO, the energy of the LUMO ELUMO, the hardness HD, and the difference between EHOMO and EHOMO-1. Results: A wide range of SVM expts. were performed using the dot, polynomial, radial basis function, neural, and anova kernels. The results obtained for the classification of PAH carcinogenicity demonstrate that the performances of SVM depend strongly on the kernel type and various parameters that control the kernel shape. The best prediction results were obtained with the radial basis function kernel with γ = 0.5, the anova kernel with γ =

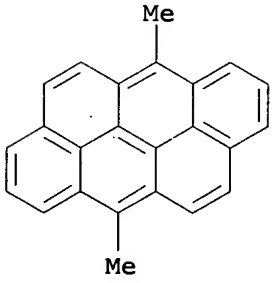
0.5 and d = 1, and the anova kernel with γ = 0.5 and d = 2. In the first case, from 34 carcinogenic compds., 28 were correctly classified, while from 44 non-carcinogenic compds., 40 were correctly classified. Conclusions. SAR models for predicting the carcinogenic hazard can benefit from the use of support vector machines, which determine a maximum separating hyperplane between carcinogenic and non-carcinogenic compds. The solution of the SVM model is a unique hyperplane which can be computed very fast, but the classification results heavily depend on the kernel type and structural descriptors. Extensive cross-validation tests should be made to find the kernel with the optimum predictive power.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(support vector machine classification of carcinogenic activity of polycyclic aromatic hydrocarbons)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)

IT 50-32-8, Benzo[3,4]pyrene, biological studies 53-70-3, Dibenz(1,2;5,6)anthracene 56-55-3, Benz[1,2]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[3,4;5,6]phenanthrene 189-55-9, Dibenzo[3,4;9,10]pyrene 189-64-0, Dibenzo[3,4;8,9]pyrene 190-99-8, Dibenzo[1,2;5,6]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Anthanthrene 191-30-0, Dibenzo[1,2;3,4]pyrene 192-65-4, Dibenzo[3,4;6,7]pyrene

192-97-2, Benzo[1,2]pyrene 194-69-4, Dibenzo[1,2;5,6]phenanthrene 195-19-7, Benzo[3,4]phenanthrene 196-78-1, Dibenzo[1,2;3,4]phenanthrene 213-46-7, Picene 215-26-9, Tribenz(1,2;3,4;5,6)anthracene 215-58-7, Dibenz(1,2;3,4)anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 224-41-9, Dibenz(1,2;7,8)anthracene 226-88-0, Benzo[1,2]naphthacene 239-98-5, Benzo[1,2]pentacene 316-14-3, 6-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5, 1-Methylbenzo[c]phenanthrene 4076-40-8, 4-Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene 16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene 60032-75-9, Tribenzo[3,4;6,7;8,9]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(support vector machine classification of carcinogenic activity of polycyclic aromatic hydrocarbons)

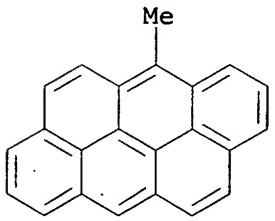
L33 ANSWER 7 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:582202 Document No. 137:181007 QSAR carcinogenic study of methylated polycyclic aromatic hydrocarbons based on topological descriptors derived from distance matrices and correlation weights of local graph invariants. Marino, Damian J. G.; Peruzzo, Pablo J.; Castro, Eduardo A.; Toropov, Andrey A. (C.I.M.A., Departamento de Quimica, Facultad de Ciencias Exactas, UNLP, La Plata, 1900, Argent.). Internet Electronic Journal of Molecular Design [online computer file], 1(3), 115-133 (English) 2002. CODEN: IEJMAT. ISSN: 1538-6414. URL: http://biochempress.com/iejmd_2001_1_0115.pdf Publisher: BioChem Press.

AB A quant. structure-activity study for the carcinogenic activity of methylated polycyclic aromatic hydrocarbons is made on the basis of topol. mol. descriptors derived from distance matrixes and optimized correlation wts. of local graph invariants. The multilinear regression equations allow us to predict correctly the carcinogenic activity of this set of compds. Comparison with results derived from other theor. studies show a quite satisfactory behavior of the present method. Some possible future extensions are pointed out.

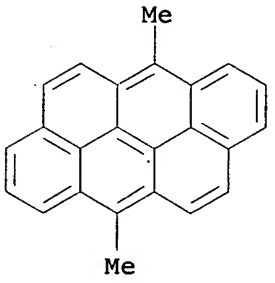
IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene

RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(QSAR carcinogenic study of methylated polycyclic aromatic hydrocarbons based on topol. descriptors derived from distance matrixes and correlation wts. of local graph invariants)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT 50-32-8D, Benzo[a]pyrene, Me derivs. 56-55-3D, Benz[a]anthracene, Me derivs. 57-97-6, 7,12-Dimethylbenz[a]anthracene 195-19-7D, Benzo[c]phenanthrene, Me derivs. 316-14-3, 6-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5, 1-Methylbenzo[c]phenanthrene 4076-40-8, 4-Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene

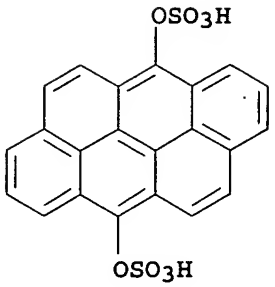
16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene 31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene 70644-19-8, 9-Methylbenzo[a]pyrene 82721-25-3, 6,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(QSAR carcinogenic study of methylated polycyclic aromatic hydrocarbons based on topol. descriptors derived from distance matrixes and correlation wts. of local graph invariants)

L33 ANSWER 8 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:555590 Document No. 137:110641 Water-based jet printing inks and ink fixation method. Sakai, Taisaburo (Japan). PCT Int. Appl. WO 2002057377 A1 20020725, 40 pp. DESIGNATED STATES: W: DE, US; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (Japanese). CODEN: PIXXD2. APPLICATION: WO 2001-JP370 20010119.

AB A fixation method for inks containing a soluble vat dye comprises printing a paper with the inks by jet printing and then irradiating the ink dots on the paper with a laser light to insolubilize the colorant and thereby fix the inks. An ink-jet print can be obtained which is free from ink dot blurring, has a bright color, and is comparable in durability (water resistance and light resistance) to conventional printed matters.

IT **1324-18-1 1324-23-8 1324-23-8D**, potassium or lithium salt **4378-58-9D**, potassium or lithium salt **10290-03-6 30756-44-6D**, potassium or lithium salt
RL: TEM (Technical or engineered material use); USES (Uses)
(water-based jet printing inks containing soluble vat dyes and ink fixation by laser irradiation)

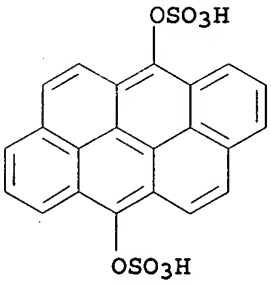
RN 1324-18-1 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate), disodium salt (7CI, 8CI, 9CI) (CA INDEX NAME)



2 (D1—O—Me)

●2 Na

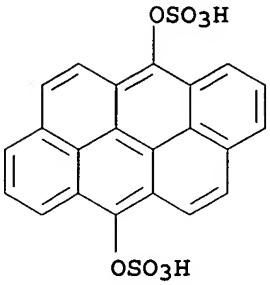
RN 1324-23-8 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, diethoxy-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



2 (D1—O—Et)

●2 Na

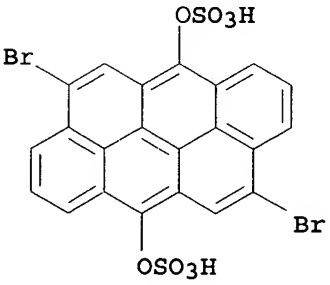
RN 1324-23-8 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, diethoxy-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



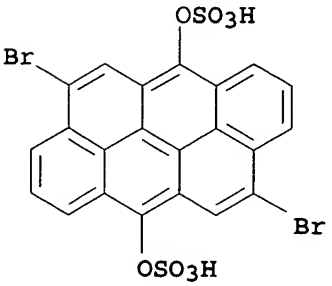
2 (D1—O—Et)

●2 Na

RN 4378-58-9 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) (8CI, 9CI) (CA INDEX NAME)

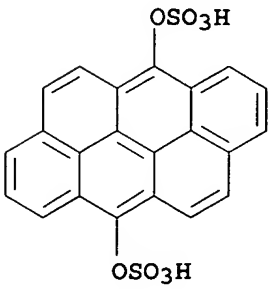


RN 10290-03-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



●2 Na

RN 30756-44-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate) (9CI) (CA INDEX NAME)



2 (D1—O—Me)

IC ICM C09D011-00
ICS B41M005-00; B41J002-01
CC 42-12 (Coatings, Inks, and Related Products)
Section cross-reference(s): 41
IT **1324-18-1 1324-23-8 1324-23-8D,** potassium or lithium salt 1324-57-8 1324-72-7 2519-28-0 2538-84-3 2678-71-9D, potassium or lithium salt 2702-33-2 2747-19-5 3564-70-3 3875-70-5 3875-72-7 3956-62-5 4086-05-9 4335-00-6D, potassium or lithium salt **4378-58-9D**, potassium or lithium salt 4388-08-3D, potassium or lithium salt 4388-09-4D, potassium or lithium salt 4388-10-7D, potassium or lithium salt 4388-11-8D, potassium or lithium salt 4388-12-9D, potassium or lithium salt 4425-36-9 4471-37-8 4478-02-8D, potassium or lithium salt 4568-45-0D, potassium or lithium salt 4735-07-3 5156-38-7 6054-59-7 6252-77-3D, potassium or lithium salt 6252-81-9D, potassium or lithium salt 6371-33-1D, potassium or lithium salt 6371-36-4D, potassium or lithium salt 6371-52-4D, potassium or lithium salt 6406-11-7D, potassium or lithium salt 6406-16-2D, potassium or lithium salt 6406-17-3D, potassium or lithium salt 6472-76-0D, potassium or lithium salt 6487-09-8 6527-57-7D, potassium or lithium salt 6527-58-8D, potassium or lithium salt 6534-24-3D, potassium or lithium salt 6535-53-1 6536-59-0D, potassium or lithium salt 6536-61-4D, potassium or lithium salt 6537-70-8 6548-41-0D, potassium or lithium salt 6711-18-8 6711-83-7 6772-33-4D, potassium or lithium salt 6787-78-6D, potassium or lithium salt 6897-40-1D, potassium or lithium salt 6897-42-3D, potassium or lithium salt 10126-84-8 10126-85-9 10126-86-0 10126-87-1 10126-90-6 10126-91-7 10126-92-8 10126-97-3 10126-99-5 10127-00-1 10127-24-9 10134-35-7 10169-28-5 10169-29-6 10169-52-5 10241-20-0 **10290-03-6** 13109-68-7 23594-58-3 25666-23-3D, potassium or lithium salt 25740-96-9D, potassium or lithium salt 25740-98-1D, potassium or lithium salt 25849-14-3D, potassium or lithium salt 27758-22-1D, potassium or lithium salt **30756-44-6D**, potassium or lithium salt 32033-20-8D, potassium or lithium salt 32073-36-2D, potassium or lithium salt 94086-99-4D, potassium or lithium salt 104353-05-1D, potassium or lithium salt 106383-49-7 107442-68-2D, potassium or lithium salt 121991-36-4D, potassium or lithium salt 217189-48-5 217189-49-6

217189-50-9 217189-51-0 217189-52-1 379738-09-7D, potassium or lithium salt 379738-10-0D, potassium or lithium salt 379738-11-1D, potassium or lithium salt 379738-12-2D, potassium or lithium salt 379738-13-3D, potassium or lithium salt 379738-14-4D, potassium or lithium salt 379738-15-5D, potassium or lithium salt 379738-16-6D, potassium or lithium salt 379738-17-7D, potassium or lithium salt 379738-18-8D, potassium or lithium salt 379738-20-2D, potassium or lithium salt 443304-08-3 443304-09-4 443304-10-7 443304-11-8 443753-18-2D, potassium or lithium salt

RL: TEM (Technical or engineered material use); USES (Uses)
(water-based jet printing inks containing soluble vat dyes and ink fixation by laser irradiation)

L33 ANSWER 10 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

2001:900438 Document No. 136:38976 Ink fixation method for ink-jet ink. Sakai, Taizaburo (Japan). Jpn. Kokai Tokkyo Koho JP 2001342383 A2 20011214, 58 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2000-50312 20000122.

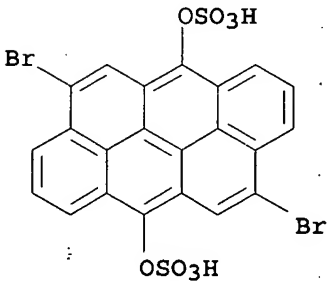
AB The method comprises ink-jet recording with a ink containing water-soluble dye and then irradiating the ink-dot with laser to convert the ink insol.

IT **4378-58-9D**, salts **30756-44-6D**, salts

RL: PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(ink fixation with laser radiation after recording)

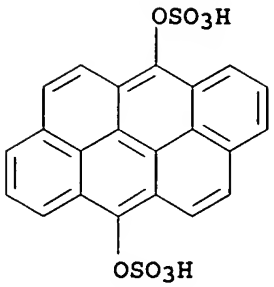
RN 4378-58-9 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) (8CI, 9CI) (CA INDEX NAME)



RN 30756-44-6 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate) (9CI) (CA INDEX NAME)



2 (D1—O—Me)

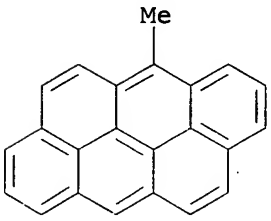
IC ICM C09D011-00
ICS B41J002-01; B41M005-00
CC 42-12 (Coatings, Inks, and Related Products)
IT 1324-22-7D, salts 2678-71-9D, salts 4335-00-6D, salts
4378-58-9D, salts 4388-09-4D, salts 4388-10-7D, salts
4388-11-8D, salts 4388-12-9D, salts 4478-02-8D, salts
4568-45-0D, salts 6252-77-3D, salts 6252-81-9D, salts
6371-33-1D, salts 6371-36-4D, salts 6371-52-4D, salts
6406-11-7D, salts 6406-16-2D, salts 6406-17-3D, salts
6472-76-0D, salts 6527-57-7D, salts 6527-58-8D, salts
6534-24-3D, salts 6536-59-0D, salts 6536-61-4D, salts
6548-41-0D, salts 6772-33-4D, salts 6787-78-6D, salts
6897-40-1D, salts 6897-42-3D, salts 25666-23-3D, salts
25740-96-9D, salts 25849-14-3D, salts 27758-22-1D, salts
30638-08-5D, Cobalt phthalocyaninesulfonate, salts
30756-44-6D, salts 32033-20-8D, salts 94086-99-4D, salts
107442-68-2D, salts 121991-36-4D, salts 379738-09-7D, salts
379738-10-0D, salts 379738-11-1D, salts 379738-12-2D, salts
379738-13-3D, salts 379738-14-4D, salts 379738-15-5D, salts
379738-16-6D, salts 379738-17-7D, salts 379738-18-8D, salts
379738-20-2D, salts
RL: PEP (Physical, engineering or chemical process); TEM (Technical or engineered material use); PROC (Process); USES (Uses)
(ink fixation with laser radiation after recording)

L33 ANSWER 11 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2001:173570 Document No. 135:42074 Structure-carcinogenic activity relationship studies of polycyclic aromatic hydrocarbons (PAHs) with pattern-recognition methods. Vendrame, R.; Braga, R. S.; Takahata, Y.; Galvao, D. S. (Instituto de Fisica Gleb Wataghin, CP 6154, CEP 13083-970, UNICAMP, Sao Paulo, Campinas, Brazil). THEOCHEM, 539, 253-265 (English) 2001. CODEN: THEODJ. ISSN: 0166-1280. Publisher: Elsevier Science B.V..
AB Recently a new methodol. to identify the carcinogenic activity of polycyclic aromatic hydrocarbons (PAHs) was proposed. This methodol. named electronic indexes methodol. (EIM) is based on the use of local d. of states (LDOS) calcns. In this work the authors perform a comparative study of this methodol. with principal component anal. (PCA) and artificial neural networks (ANN). All the physicochem. descriptors were calculated from the mol. eigenstates/spectra obtained through the well-known semi-empirical method parametric method 3 (PM3). PCA and ANN results show that EIM descriptors are relevant to identify the carcinogenic activity of methylated and

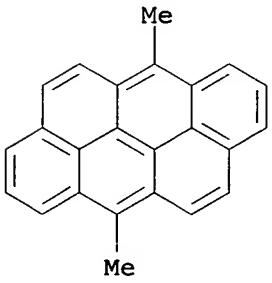
non-methylated PAHs. Also, the authors show that the combined use of these distinct methodologies can be an efficient and powerful tool in the structure-activity studies of PAHs or other organic compds. The authors have studied 81 methylated and non-methylated PAHs, and the authors' study shows that with the use of these methods it is possible to predict correctly the PAHs' carcinogenic activity with high accuracy (.apprx.80%).

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(structure-carcinogenic activity relationship studies of polycyclic aromatic hydrocarbons with pattern-recognition methods)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)

IT 50-32-8, Benzo[3,4]pyrene, biological studies 53-70-3, Dibenzo[1,2:5,6]anthracene 56-55-3, Benzo[1,2]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[3,4:5,6]phenanthrene 189-55-9, Dibenzo[3,4:9,10]pyrene 189-64-0, Dibenzo[3,4:8,9]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Anthanthrene 191-30-0, Dibenzo[1,2:3,4]pyrene 192-47-2, Dibenzo[h,rst]pentaphene 192-51-8, Dibenzo[fg,op]naphthacene 192-65-4, Naphtho[1,2,3,4-def]chrysene 192-97-2, Benzo[1,2]pyrene 194-69-4, Dibenzo[1,2:5,6]phenanthrene 195-19-7, Benzo[3,4]phenanthrene 196-42-9, Naphtho[2,1,8-qra]naphthacene 196-78-1, Dibenzo[1,2:3,4]phenanthrene 213-46-7, Picene

215-26-9, Naphtho[1,2-b]triphenylene 215-58-7, Dibenzo[1,2:3,4]anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 222-54-8, Benzo[c]pentaphene 224-41-9, Dibenzo[1,2:7,8]anthracene 226-88-0, Benzo[1,2]naphthacene 239-98-5, Benzo[1,2]pentacene 316-14-3, 6-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5, 1-Methylbenzo[c]phenanthrene 4076-40-8, 4-Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene 16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene 31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 60032-75-9, Tribenzo[b,def,p]chrysene 63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene 70644-19-8, 9-Methylbenzo[a]pyrene 82721-25-3, 6,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(structure-carcinogenic activity relationship studies of polycyclic aromatic hydrocarbons with pattern-recognition methods)

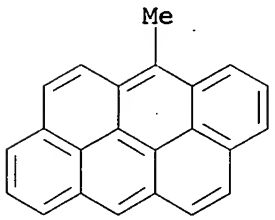
L33 ANSWER 12 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2001:137879 Document No. 134:321916 Structure-toxicity relationships of polycyclic aromatic hydrocarbons using molecular quantum similarity. Gallegos, Ana; Robert, David; Girones, Xavier; Carbo-Dorca, Ramon (Institute of Computational Chemistry, University of Girona, Catalonia, E-17071, Spain). Journal of Computer-Aided Molecular Design, 15(1), 67-80 (English) 2001. CODEN: JCADEQ. ISSN: 0920-654X. Publisher: Kluwer Academic Publishers.

AB The establishment of quant. structure-activity relationship (QSAR) models for the toxicity of polycyclic aromatic hydrocarbons (PAHs) is described. Two properties, in vitro percutaneous absorption in rat skin and discrete levels of carcinogenic activity, are examined using mol. quantum similarity measures (MQSM). The results show that MQSM produces comparable, or even better, results than other approaches using physicochem., topol. and quantum-chemical mol. descriptors. Furthermore, a careful anal. puts into evidence that most of the information characterized by the original descriptors is in fact contained in the mol. d. functions, the basis of MQSM. The present

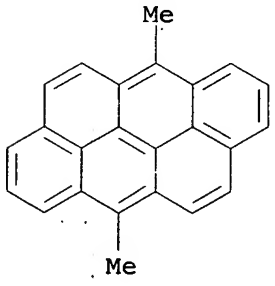
paper, together with several other reported by our laboratory, proves that MQSM might be appropriate theor. tools for QSAR and computer-aided drug design, comparable to other highly predictive QSAR methodologies.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(structure-toxicity relationships of polycyclic aromatic hydrocarbons using mol. quantum similarity)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)

IT 50-32-8, Benzo[a]pyrene, biological studies 53-70-3, Dibenz[a,h]anthracene 56-49-5, 3-Methylcholanthrene 56-55-3, Benzo[a]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 86-73-7, Fluorene 91-20-3, Naphthalene, biological studies 120-12-7, Anthracene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[3,4:5,6]phenanthrene 189-55-9, Benzo[rst]pentaphene 189-64-0, Dibenzo[3,4:8,9]pyrene 190-99-8, Dibenzo[1,2:5,6]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Dibenzo[def,mno]chrysene 191-30-0, Dibenzo[a,l]pyrene 192-47-2, Dibenzo[h,rst]pentaphene 192-65-4, Naphtho[1,2,3,4-def]chrysene 192-97-2, Benzo[e]pyrene 193-39-5, Indeno[1,2,3-cd]pyrene 194-69-4, Dibenzo[1,2:5,6]phenanthrene 195-19-7, Benzo[c]phenanthrene 196-78-1, Dibenzo[1,2:3,4]phenanthrene 198-55-0, Perylene 203-64-5, 4H-Cyclopenta[def]phenanthrene 206-44-0, Fluoranthene 207-08-9, Benzo[k]fluoranthene 213-46-7,

Picene 215-26-9, Naphtho[1,2-b]triphenylene 215-58-7,
2,3-Benzotriphenylene 217-59-4, Triphenylene 218-01-9, Chrysene
222-54-8, Benzo[c]pentaphene 224-41-9, Dibenzo[1,2:7,8]anthracene
226-88-0, Benzo[1,2]naphthacene 238-84-6, 1,2-Benzofluorene
239-98-5, Benzo[1,2]pentacene 243-17-4, 2,3-Benzofluorene
316-14-3, 6-Methylbenz[a]anthracene 316-51-8, 3,9-
Dimethylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene
483-65-8, 1-Methyl-7-isopropylphenanthrene 568-81-0,
6,12-Dimethylbenz[a]anthracene 602-55-1, 9-Phenylanthracene
610-48-0, 1-Methylanthracene 613-12-7, 2-Methylanthracene
613-31-0, 9,10-Dihydroanthracene 652-04-0, 5-
Methylbenzo[c]phenanthrene 776-35-2, 9,10-Dihydrophenanthrene
789-24-2, 9-Phenylfluorene 832-69-9, 1-Methylphenanthrene
1499-10-1, 9,10-Diphenylanthracene 1572-46-9, 9-Benzylfluorene
1576-67-6, 3,6-Dimethylphenanthrene 1705-85-7, 6-Methylchrysene
1730-37-6, 1-Methylfluorene 1732-13-4, 1,2,3,6,7,8-Hexahydropyrene
1836-87-9, 9-Benzylidenefluorene 2294-82-8, 9-Ethylfluorene
2319-96-2, 5-Methylbenz[a]anthracene 2381-15-9,
10-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene
2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene
2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2,
6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene
2422-79-9, 12-Methylbenz[a]anthracene 2444-68-0, 9-Vinylanthracene
2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2,
2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene
2531-84-2, 2-Methylphenanthrene 2541-69-7, 7-
Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene
2732-58-3, 6-Ethylchrysene 3353-12-6, 4-Methylpyrene 3442-78-2,
2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5,
1-Methylbenzo[c]phenanthrene 4076-40-8, 4-
Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene
6111-78-0, 11-Methylbenz[a]anthracene 7198-87-0,
5,6-Dihydro-4H-dibenz[a,kl]anthracene 7468-93-1 16757-80-5,
11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene
16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8,
4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene
16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1,
1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene
16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4,
4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene
16757-91-8, 3,6-Dimethylbenzo[a]pyrene 17088-22-1, 3-Ethylpyrene
18153-42-9, 9-(m-Tolyl)fluorene 18153-43-0, 9-(p-Tolyl)fluorene
18801-00-8, 2-(tert-Butyl)anthracene 20496-16-6,
3-Ethylfluoranthene 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene
31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**,
6-Methylanthanthrene 33543-31-6, 2-Methylfluoranthene
40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**,
6,12-Dimethylanthanthrene 52251-71-5, 2-Ethylanthracene
56142-13-3, Butylpyrene 60032-75-9, Tribenzo[b,def,p]chrysene
63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0,
7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene
63104-33-6, 7,10-Dimethylbenzo[a]pyrene 70644-19-8,
9-Methylbenzo[a]pyrene 82721-25-3, 6,10-Dimethylbenzo[a]pyrene
221269-46-1, 9-Cinnamylfluorene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL
(Biological study)
(structure-toxicity relationships of polycyclic aromatic
hydrocarbons using mol. quantum similarity)

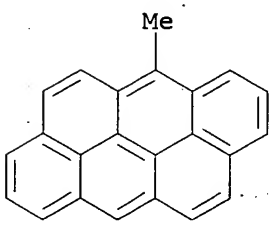
L33 ANSWER 13 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

2000:746040 Document No. 134:218063 Identifying carcinogenic activity of methylated and non-methylated polycyclic aromatic hydrocarbons (PAHs) through electronic and topological indices. Braga, R. S.; Barone, P. M. V. B.; Galvao, D. S. (Instituto de Fisica, Universidade Estadual de Campinas - UNICAMP, Campinas, CEP 13081-970, Brazil). Brazilian Journal of Physics, 30(3), 560-568 (English) 2000. CODEN: BJPHE6. ISSN: 0103-9733. Publisher: Sociedade Brasileira de Fisica.

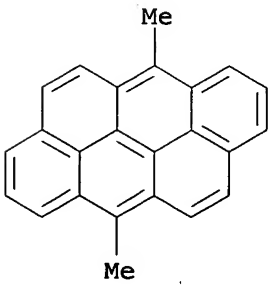
AB Polycyclic aromatic hydrocarbons (PAHs) are a class of planar mols., abundant in urban environment, which can induce chemical carcinogenesis. Their carcinogenic power varies in a large range, from very strong carcinogens to inactive ones. In a previous study, the authors proposed a methodol. to identify the PAHs carcinogenic activity exploring electronic and topol. indexes. In the present work, the authors show that it is possible to simplify that methodol. and expand its applicability to include methylated PAHs compds. Using very simple rules, the authors can predict their carcinogenic activity with high accuracy (≈ 89%).

IT **31927-64-7 41217-05-4**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenic activity of methylated and non-methylated polycyclic aromatic hydrocarbons (PAHs) identification through electronic and topol. indexes)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-1 (Toxicology)

IT 50-32-8, Benzo[a]pyrene, biological studies 53-70-3, Dibenz[a,h]anthracene 56-55-3, Benz[a]anthracene 57-97-6 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene,

biological studies 91-20-3, Naphthalene, biological studies
129-00-0, Pyrene, biological studies 188-52-3,
Dibenzo[c,g]phenanthrene 189-55-9, Benzo[rst]pentaphene
189-64-0, Dibenzo[b,def]chrysene 191-07-1, Coronene 191-24-2,
Benzo[ghi]perylene 191-26-4, Dibenzo[def,mno]chrysene 191-30-0,
Dibenzo[def,p]chrysene 192-47-2, Dibenzo[h,rst]pentaphene
192-51-8, Dibenzo[fg,op]naphthacene 192-65-4, Naphtho[1,2,3,4-
def]chrysene 192-97-2, Benzo[e]pyrene 194-69-4, Benzo[c]chrysene
195-19-7, Benzo[c]phenanthrene 196-42-9, Naphtho[2,1,8-
qra]naphthacene 196-78-1, Benzo[g]chrysene 213-46-7, Picene
215-26-9, Naphtho[1,2-b]triphenylene 215-58-7,
Benzo[b]triphenylene 217-59-4, Triphenylene 218-01-9, Chrysene
222-54-8, Benzo[c]pentaphene 224-41-9, Dibenz[a,j]anthracene
226-88-0, Benzo[a]naphthacene 239-98-5, Benzo[a]pentacene
316-14-3 317-64-6 568-81-0 652-04-0 1705-85-7 2319-96-2
2381-16-0 2381-19-3 2381-21-7 2381-31-9 2381-34-2
2381-39-7 2422-79-9 2498-75-1 2498-76-2 2498-77-3
2541-69-7 2606-85-1 3353-12-6 3442-78-2 3697-24-3
4076-39-5 4076-40-8 4514-19-6 6111-78-0 16757-80-5
16757-81-6 16757-82-7 16757-83-8 16757-84-9 16757-85-0
16757-86-1 16757-87-2 16757-88-3 16757-89-4 16757-90-7
16757-91-8 20627-34-3 31647-36-6 **31927-64-7**
40568-90-9 **41217-05-4** 60032-75-9,
Tribenzo[b,def,p]chrysene 63041-76-9 63041-77-0 63104-32-5
63104-33-6 70644-19-8 82721-25-3
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenic activity of methylated and non-methylated polycyclic aromatic hydrocarbons (PAHs) identification through electronic and topol. indexes)

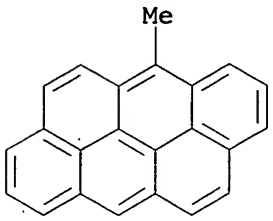
L33 ANSWER 14 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1999:663090 Document No. 132:9850 Structure-Activity Relationship Studies of Carcinogenic Activity of Polycyclic Aromatic Hydrocarbons Using Calculated Molecular Descriptors with Principal Component Analysis and Neural Network Methods. Vendrame, R.; Braga, R. S.; Takahata, Y.; Galvao, D. S. (Instituto de Fisica Gleb Wataghin and Instituto de Quimica, UNICAMP, Campinas, 13083-970, Brazil). Journal of Chemical Information and Computer Sciences, 39(6), 1094-1104 (English) 1999. CODEN: JCISD8. ISSN: 0095-2338. Publisher: American Chemical Society.

AB Recently a new methodol. based on local d. of state (LDOS) calcns. using topol. and semiempirical methods was proposed to identify the carcinogenic activity of polycyclic aromatic hydrocarbons (PAHs). In this work we perform a comparative study of this methodol. with principal component anal. (PCA) and neural networks (NN). The PCA and NN results show that LDOS quantum chemical descriptors are relevant descriptors to identify the carcinogenic activity of methylated and non-methylated PAHs. Also, we show that the combination of these distinct methodologies can be an efficient and powerful tool in the structure-activity studies of PAHs compds. We have studied 81 methylated and non-methylated PAHs, and our study shows that with the use of these methods it is possible to correctly predict the carcinogenic activity of PAHs with accuracy higher than 80%.

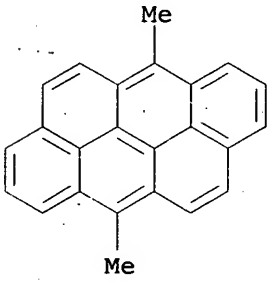
IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**, 6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(structure-activity relationship studies of carcinogenic activity of polycyclic aromatic hydrocarbons using calculated mol. descriptors

with principal component anal. and neural network methods)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT 50-32-8, Benzo[3,4]pyrene, biological studies 53-70-3, Dibenzo[1,2:5,6]anthracene 56-55-3, Benzo[1,2]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[3,4:5,6]phenanthrene 189-55-9, Dibenzo[3,4:9,10]pyrene 189-64-0, Dibenzo[3,4:8,9]pyrene 190-99-8, Dibenzo[1,2:5,6]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Anthanthrene 191-30-0, Dibenzo[1,2:3,4]pyrene 192-47-2, Dibenzo[h,rst]pentaphene 192-65-4, Naphtho[1,2,3,4-def]chrysene 192-97-2, Benzo[1,2]pyrene 194-69-4, Dibenzo[1,2:5,6]phenanthrene 195-19-7, Benzo[3,4]phenanthrene 196-42-9, Naphtho[2,1,8-qra]naphthacene 196-78-1, Dibenzo[1,2:3,4]phenanthrene 213-46-7, Picene 215-26-9, Naphtho[1,2-b]triphenylene 215-58-7, Dibenzo[1,2:3,4]anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 222-54-8, Benzo[c]pentaphene 224-41-9, Dibenzo[1,2:7,8]anthracene 226-88-0, Benzo[1,2]naphthacene 239-98-5, Benzo[1,2]pentacene 316-14-3, 6-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7,

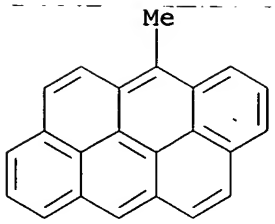
6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene
2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2,
2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene
2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1,
2-Methylbenzo[c]phenanthrene 3353-12-6, 4-Methylpyrene
3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5,
1-Methylbenzo[c]phenanthrene 4076-40-8, 4-
Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene
6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5,
11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene
16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8,
4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene
16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1,
1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene
16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4,
4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene
16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3,
6,8,12-Trimethylbenz[a]anthracene 31647-36-6, 5-
Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene
40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**,
6,12-Dimethylanthanthrene 60032-75-9, Tribenzo[b,def,p]chrysene
63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0,
7-Methylbenzo[a]pyrene 63104-32-5, 10=Methylbenzo[a]pyrene
63104-33-6, 7,10-Dimethylbenzo[a]pyrene 70644-19-8,
9-Methylbenzo[a]pyrene 82721-25-3, 6,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse èffect, including toxicity); PRP (Properties); BIOL (Biological study)
(structure-activity relationship studies of carcinogenic activity of polycyclic aromatic hydrocarbons using calculated mol. descriptors with principal component anal. and neural network methods)

L33 ANSWER 15 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1999:308470 Document No. 131:98732 Identifying carcinogenic activity of methylated polycyclic aromatic hydrocarbons (PAHs). Braga, R. S.; Barone, P. M. V. B.; Galvao, D. S. (Instituto de Fisica, Universidade Estadual de Campinas - UNICAMP, Campinas, 13081-970, Brazil). THEOCHEM, 464(1-3), 257-266 (English) 1999. CODEN: THEODJ. ISSN: 0166-1280. Publisher: Elsevier Science B.V..

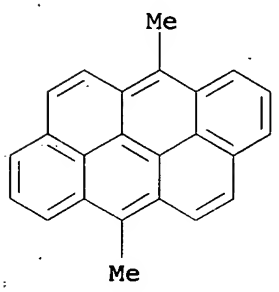
AB Polycyclic aromatic hydrocarbons (PAHs) are a class of planar mols. that can induce chemical carcinogenesis. Their carcinogenic power vary in a large range, from the very strong carcinogens to the inactive ones. Recently a new methodol. was proposed (using the topol. simple Huckel theory) to group and identify PAHs carcinogenic activity in terms of very simple rules based on the concept of electronic local d. of states over specific mol. regions. In the present work we have extended this study to include methylated compds. Our results show that the previous methodol. can also. be simplified and successfully used to predict the carcinogenic activity of methylated PAHs.

IT **31927-64-7**, 6-Methylanthanthrene **41217-05-4**,
6,12-Dimethylanthanthrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(identifying carcinogenic activity of methylated polycyclic aromatic hydrocarbons)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



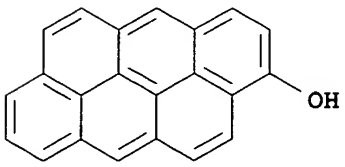
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT 50-32-8, Benzo[3,4]pyrene, biological studies 53-70-3, Dibenzo[1,2:5,6]anthracene 56-55-3, Benzo[1,2]anthracene 57-97-6, 7,12-Dimethylbenz[a]anthracene 71-43-2, Benzene, biological studies 85-01-8, Phenanthrene, biological studies 91-20-3, Naphthalene, biological studies 129-00-0, Pyrene, biological studies 188-52-3, Dibenzo[3,4:5,6]phenanthrene 189-55-9, Dibenzo[3,4:9,10]pyrene 189-64-0, Dibenzo[3,4:8,9]pyrene 191-07-1, Coronene 191-24-2, Benzo[ghi]perylene 191-26-4, Anthanthrene 191-30-0, Dibenzo{1,2:3,4]pyrene 192-47-2, Dibenzo[h,rst]pentaphene 192-51-8, Dibenzo[fg,op]naphthacene 192-65-4, Naphtho[1,2,3,4-def]chrysene 192-97-2, Benzo[1,2]pyrene 194-69-4, Dibenzo[1,2:5,6]phenanthrene 195-19-7, Benzo[3,4]phenanthrene 196-42-9, Naphtho[2,1,8-qra]naphthacene 196-78-1, Dibenzo[1,2:3,4]phenanthrene 213-46-7, Picene 215-26-9, Naphtho[1,2-b]triphenylene 215-58-7, Dibenzo[1,2:3,4]anthracene 217-59-4, Triphenylene 218-01-9, Chrysene 222-54-8, Benzo[c]pentaphene 224-41-9, Dibenzo[1,2:7,8]anthracene 226-88-0, Benzo[1,2]naphthacene 239-98-5, Benzo[1,2]pentacene 316-14-3, 6-Methylbenz[a]anthracene 317-64-6, 6,8-Dimethylbenz[a]anthracene 568-81-0, 6,12-Dimethylbenz[a]anthracene 652-04-0, 5-Methylbenzo[c]phenanthrene 1705-85-7, 6-Methylchrysene 2319-96-2, 5-Methylbenz[a]anthracene 2381-16-0, 9-Methylbenz[a]anthracene 2381-19-3, 3-Methylbenzo[c]phenanthrene 2381-21-7, 1-Methylpyrene 2381-31-9, 8-Methylbenz[a]anthracene 2381-34-2, 6-Methylbenzo[c]phenanthrene 2381-39-7, 6-Methylbenzo[a]pyrene 2422-79-9, 12-Methylbenz[a]anthracene 2498-75-1, 3-Methylbenz[a]anthracene 2498-76-2, 2-Methylbenz[a]anthracene 2498-77-3, 1-Methylbenz[a]anthracene 2541-69-7, 7-Methylbenz[a]anthracene 2606-85-1, 2-Methylbenzo[c]phenanthrene 3353-12-6, 4-Methylpyrene 3442-78-2, 2-Methylpyrene 3697-24-3, 5-Methylchrysene 4076-39-5,

1-Methylbenzo[c]phenanthrene 4076-40-8, 4-Methylbenzo[c]phenanthrene 4514-19-6, 12-Methylbenzo[a]pyrene 6111-78-0, 11-Methylbenz[a]anthracene 16757-80-5, 11-Methylbenzo[a]pyrene 16757-81-6, 3-Methylbenzo[a]pyrene 16757-82-7, 2-Methylbenzo[a]pyrene 16757-83-8, 4-Methylbenzo[a]pyrene 16757-84-9, 3,12-Dimethylbenzo[a]pyrene 16757-85-0, 1,2-Dimethylbenzo[a]pyrene 16757-86-1, 1,3-Dimethylbenzo[a]pyrene 16757-87-2, 2,3-Dimethylbenzo[a]pyrene 16757-88-3, 1,4-Dimethylbenzo[a]pyrene 16757-89-4, 4,5-Dimethylbenzo[a]pyrene 16757-90-7, 1,6-Dimethylbenzo[a]pyrene 16757-91-8, 3,6-Dimethylbenzo[a]pyrene 20627-34-3, 6,8,12-Trimethylbenz[a]anthracene 31647-36-6, 5-Methylbenzo[a]pyrene **31927-64-7**, 6-Methylanthanthrene 40568-90-9, 1-Methylbenzo[a]pyrene **41217-05-4**, 6,12-Dimethylanthanthrene 60032-75-9, Tribenzo[b,def,p]chrysene 63041-76-9, 8-Methylbenzo[a]pyrene 63041-77-0, 7-Methylbenzo[a]pyrene 63104-32-5, 10-Methylbenzo[a]pyrene 63104-33-6, 7,10-Dimethylbenzo[a]pyrene 70644-19-8, 9-Methylbenzo[a]pyrene 82721-25-3, 6,10-Dimethylbenzo[a]pyrene
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(identifying carcinogenic activity of methylated polycyclic aromatic hydrocarbons)

L33 ANSWER 16 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1997:326698 Document No. 127:105502 Metabolic activation of anthanthrene. Significance of stable radicals derived from its key metabolite 3-hydroxyanthanthrene. Degenhardt, Christian; Bors, Wolf; Stettmaier, Kurt; Seidel, Albrecht; Frank, Heinz; Platt, Karl L. (Institut Toxikologie, Universitat Mainz, Mainz, D-55131, Germany). Polycyclic Aromatic Compounds, 10(1-4), 85-92 (English) 1996. CODEN: PARCEO. ISSN: 1040-6638. Publisher: Gordon & Breach.
AB Anthanthrene, a hexacyclic aromatic hydrocarbon lacking the structural element of a bay-region is metabolized to 3-hydroxyanthanthrene (3-HA) and anthanthrene-3,6-quinone by rat liver microsomes. Two further metabolites of anthanthrene are also derived as metabolites of 3-HA. 3-HA forms stable radicals in the presence of horseradish peroxidase and hydrogen peroxide as revealed by ESR spectroscopy. These radical species which are also formed spontaneously from 3-HA could be responsible for the genotoxic properties of anthanthrene.
IT **192521-47-4**, Dibenzo[def,mno]chrysen-3-ol
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(metabolic activation of anthanthrene and stable radicals derived from its key metabolite hydroxyanthanthrene)
RN 192521-47-4 HCAPLUS
CN Dibenzo[def,mno]chrysen-3-ol (9CI) (CA INDEX NAME)



CC 4-6 (Toxicology)
IT **192521-47-4**, Dibenzo[def,mno]chrysen-3-ol

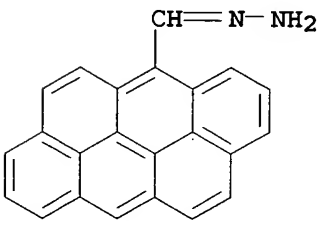
RL: BSU (Biological study, unclassified); MFM (Metabolic formation); PRP (Properties); BIOL (Biological study); FORM (Formation, nonpreparative)
(metabolic activation of anthanthrene and stable radicals derived from its key metabolite hydroxyanthanthrene)

L33 ANSWER 18 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1996:434358 Document No. 125:126623 Far-infrared emission of PAH molecules (14-40 μm): a preparation for ISO spectroscopy. Moutou, C.; Leger, A.; d'Hendecourt, L. (Institut d'Astrophysique Spatiale, Universite Paris Sud, Orsay, F-91405, Fr.). Astronomy and Astrophysics, 310(1), 297-308 (English) 1996. CODEN: AAEJAF. ISSN: 0004-6361. Publisher: Springer.

AB The authors study the absorption spectra of 40 PAH mols. (Polycyclic Aromatic Hydrocarbons) in solid matrixes, in the almost unexplored 14-75 μm range. Some accumulations of features appear among the whole sample of laboratory spectra and indicate the most probable positions of interstellar bands. After calcn. of the IR emission provided by a family of PAHs ranging from 3 to 70 Å size, it comes out that four bands are dominating and could be detected by the future IR observatory ISO, if the species involved are present at an abundance that the authors define. Their positions are 16.2, 18.2, 21.2 and 23.1 μm.

IT **179414-70-1**
RL: GFM (Geological or astronomical formation); GOC (Geological or astronomical occurrence); GPR (Geological or astronomical process); PRP (Properties); FORM (Formation, nonpreparative); OCCU (Occurrence); PROC (Process)
(far-IR emission of PAH mols. (14-40 μm): a preparation for ISO spectroscopy)

RN 179414-70-1 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-carboxaldehyde, hydrazone (9CI) (CA INDEX NAME)



CC 73-9 (Optical, Electron, and Mass Spectroscopy and Other Related Properties)

IT 85-01-8, Phenanthrene, properties 129-00-0, Pyrene, properties 188-94-3, Diindeno[1,2,3-cd:1',2',3'-lm]perylene 188-96-5, Dibenzo[cd,lm]perylene 190-24-9, Hexabenzo[bc,ef,hi,kl,no,qr]coronene 190-26-1, Ovalene 190-66-9, Dibenzo[a,g]coronene 190-70-5, Benzo[a]coronene 190-74-9, Naphtho[2,3-a]coronene 190-90-9 190-95-4, Dibenzo[b,pqr]perylene 191-07-1, Coronene 191-48-0, Diacenaphtho[1,2-j:1',2'-l]fluoranthene 196-02-1, Dibenzo[fg,uv]heptacene 197-69-3, Dibenzo[fg,ij]pentaphene 197-74-0, Dibenzo[fg,qr]pentacene 198-55-0, Perylene 206-44-0, Fluoranthene 517-51-1 610-48-0 779-02-2 5869-30-7, Dibenzo[b,ghi]perylene 14147-38-7, Dibenzo[de,st]pentacene 15570-45-3 17088-22-1 18801-00-8 41163-25-1 53086-28-5 54811-28-8 80277-99-2 88299-48-3 120835-83-8,

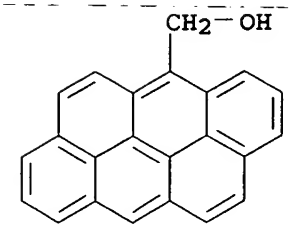
Benzo[de]naphtho[2,1,8,7-qrst]pentacene 122645-04-9 179414-65-4
179414-67-6 179414-68-7, Ovaleno[3,4-c]furan-9,11-dione
179414-69-8, Dibenzo[bc,ef]coronene-7,14-dione **179414-70-1**
179414-71-2, Benzo[h]hexaphene-1,4,16(15a)-trione
RL: GFM (Geological or astronomical formation); GOC (Geological or astronomical occurrence); GPR (Geological or astronomical process); PRP (Properties); FORM (Formation, nonpreparative); OCCU (Occurrence); PROC (Process)
(far-IR emission of PAH mols. (14-40 μm): a preparation for ISO spectroscopy)

L33 ANSWER 19 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1995:218790 Document No. 122:3290 Substance-dependent sex differences in the activation of benzylic alcohols to mutagens by hepatic sulfotransferases of the rat. Glatt, Hansruedi; Pauly, Karin; Frank, Heinz; Seidel, Albrecht; Oesch, Franz; Harvey, Ronald G.; Werle-Schneider, Gisela (Deutsches Institut fuer Ernaehrungsforschung, Potsdam-Rehbuecke, D-14558, Germany). Carcinogenesis, 15(11), 2605-11 (English) 1994. CODEN: CRNGDP. ISSN: 0143-3334. Publisher: Oxford University Press.

AB Six primary and 10 secondary benzylic alcs. derived from polycyclic aromatic hydrocarbons were tested for mutagenicity in Salmonella typhimurium TA98 in the presence of varying amts. of hepatic cytosol from adult male and female rats and 3'-phosphoadenosine-5'-phosphosulfate, the cofactor for sulfotransferases. With the exception of 1-(9-anthryl)ethanol, 4H-cyclopenta[def]-phenanthren-4-ol and 10-hydroxy-7,8,9,10-tetrahydrobenzo[a]pyrene, all the benzylic alcs. were activated to mutagens. For 1-(1-pyrenyl)ethanol (1-HEP), 1-(2-pyrenyl)ethanol (2-HEP), 6-hydroxymethylanthanthrene (6-HMAA), 2-hydroxymethylpyrene (2-HMP), 10H-indeno[1,2,7,7a-bcd]pyren-10-ol (OH-IP), 3-hydroxy-3,4-dihydrocyclopenta[cd]pyrene (3-OH-H2-CPcdP) and 1-(6-benzo[a]pyrenyl)ethanol (6-HEBP), this is the first observation of a mutagenic activity. The primary alcs. 1-hydroxymethylpyrene, 2-HMP, 9-hydroxymethylanthracene, 7-hydroxymethyl-12-methylbenz[a]anthracene and 6-hydroxymethylbenzo[a]pyrene, as well as the secondary alcs. 1-HEP and 3-OH-H2-CPcdP, were more efficiently activated by hepatic cytosol from females than by prepns. from males (2.6- to 8-fold). A further compound, 6-HEBP showed significant, but relatively weak, effects in the presence of cytosol from females, whereas it was inactive in the presence of hepatic cytosol from males. The reverse sex difference was observed in the activation of 4H-cyclopenta[def]chrysen-4-ol, the activity of cytosol from males amounting to about four times that from females. Four other compds., 2-HEP, 7-hydroxy-7,8,9,10-tetrahydrobenzo[a]pyrene, 6-HMAA and OH-IP, were activated with similar efficiency by hepatic cytosol from both sexes (<two-fold differences). The study indicates that different sulfotransferases are involve din the bioactivation of benzylic alcs., including forms preferentially expressed in females as well as forms preferentially expressed in males, and that these enzymes qual. differ in their substrate tolerance for benzylic alcs.

IT **105708-72-3**, Dibenzo[def,mno]chrysene-6-methanol
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(substance-dependent sex differences in activation of benzylic alcs. to mutagens by hepatic sulfotransferases)

RN 105708-72-3 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-methanol (9CI) (CA INDEX NAME)

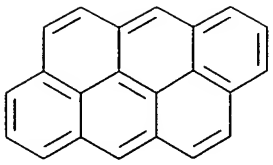


CC 4-6 (Toxicology)
IT 568-75-2, 7-Hydroxymethyl-12-methylbenz[a]anthracene 1468-95-7, 9-Hydroxymethylanthracene 6272-55-5, 7-Hydroxy-7,8,9,10-tetrahydrobenzo[a]pyrene 7512-20-1, 1-(9-Anthryl)ethanol 17573-24-9 21247-98-3, 6-Hydroxymethylbenzo[a]pyrene 24463-15-8, 1-Hydroxymethylpyrene 24471-48-5, 2-Pyrenemethanol 36271-80-4 64884-42-0, 4H-Cyclopenta[def]-phenanthren-4-ol 65954-42-9, 1-(1-Pyrenyl)ethanol 69795-73-9, 3-Hydroxy-3,4-dihydrocyclopenta[cd]pyrene 86470-99-7 **105708-72-3**, Dibenzo[def,mno]chrysene-6-methanol 143924-52-1, 4H-Cyclopenta[def]chrysen-4-ol 143924-54-3, 4H-Benzo[def]cyclopenta[mno]chrysen-4-ol
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(substance-dependent sex differences in activation of benzylic alcs. to mutagens by hepatic sulfotransferases)

L33 ANSWER 20 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1993:171038 Document No. 118:171038 Surface-active dyes and nonflocculating organic pigments for the coatings industry. 1. Behavior of surface-active dyes in organic media. Vil'ner, S. G.; Smrchek, V. A. (MNPO "NIOPIK", Moscow, USSR). Lakokrasochnye Materialy i Ikh Primenenie (2), 3-7 (Russian) 1992. CODEN: LAMAAD. ISSN: 0023-737X.
AB The degree of association depends on chemical nature and concentration of surface-active dyes (SAD), thermodn. quality of solvents, the presence of a polymer binder in the solution The ability to form assocs. (micelles) increased with increasing number of cycles in the polycyclic part of SAD and with increasing polarity of functional groups. Alkyd resins PF-060 and ML-0159 were used in the study.
IT **146622-62-0**
RL: USES (Uses)
(model compound, for surface-active dyes, behavior of, in organic media)
RN 146622-62-0 HCAPLUS
CN 1-Octadecanaminium, N,N-dimethyl-N-octadecyl-, dibenzo[def,mno]chrysenesulfonate (9CI) (CA INDEX NAME)

CM 1

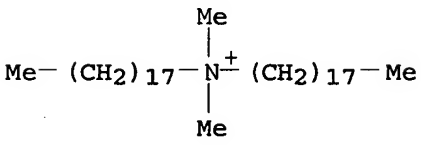
CRN 146622-61-9
CMF C22 H11 O3 S
CCI IDS



D1— SO_3^-

CM 2

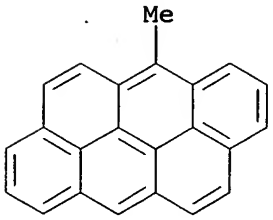
CRN 14357-21-2
CMF C38 H80 N



CC 42-8 (Coatings, Inks, and Related Products)
Section cross-reference(s): 41
IT 30753-88-9 60177-10-8 61212-60-0 81626-37-1
146622-62-0 146648-15-9 146793-76-2 146793-78-4
146793-79-5
RL: USES (Uses)
(model compound, for surface-active dyes, behavior of, in organic media)

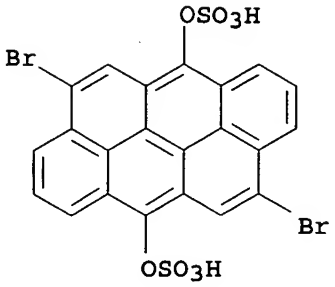
L33 ANSWER 21 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1993:24763 Document No. 118:24763 Most stable configurations of polynuclear aromatic hydrocarbon molecules in pitches via molecular modeling. Vorpagel, E. R.; Lavin, J. G. (Pioneering Res. Lab., Du Pont Fibers, Wilmington, DE, 19880-0302, USA). Carbon, 30(7), 1033-40 (English) 1992. CODEN: CRBNAH. ISSN: 0008-6223.
AB Mol. mechanics calcns. were performed on a series of polynuclear aromatic hydrocarbon mols. in various geometric arrangements and combinations. Homologous aromatic hydrocarbons associate strongly face-to-face, in a parallel shifted stack arrangement with a displacement of .apprx.4.7Å. Heteromerous aromatic hydrocarbons also prefer a shifted stack configuration 2-3 mols. high. A third or fourth mol. added to a stack will prefer to orient perpendicular to the stack, so that its face is against the edge of the stack. Me groups act to encourage stacking interactions between dissimilar aromatic hydrocarbons, with the Me groups preferring to be inside the stack and thus, having a min. effect on edge-to-edge interactions between stacks. These results support the colloidal model for the behavior of pitches.
IT **31927-64-7**
RL: MSC (Miscellaneous)
(stacked mols. of, face-to-face, interaction energy of, mol. mechanics calcn. of, pitch properties in relation to)
RN 31927-64-7 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



CC 51-10 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 22, 25, 49, 57
IT 71-43-2, Benzene, miscellaneous 120-12-7, Anthracene, miscellaneous 190-26-1, Ovalene 191-07-1, Coronene 191-26-4, Dibenzo[def,mno]chrysene 13119-86-3 **31927-64-7** 72210-95-8 145142-13-8, Tetrabenz[bc,ef,mn,pq]ovalene
RL: MSC (Miscellaneous)
(stacked mols. of, face-to-face, interaction energy of, mol. mechanics calcn. of, pitch properties in relation to)

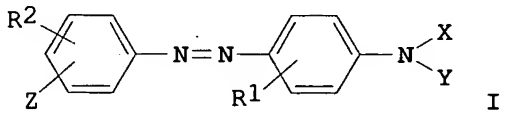
L33 ANSWER 22 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1992:513404 Document No. 117:113404 Dyeing of wool with the aim of better light fastness at high temperatures. Valldeperas, Jose; Cegarra, Jose; Gacen, Joaquin; Navarro, J. A. (Polytech. Univ. Catalunya, Spain). Melliand Textilberichte, 73(4), E151-E153, 345-8 (English/German) 1992. CODEN: MTIRDL. ISSN: 0341-0781.
AB Several deep shades of Indigosol dyes have a sufficient lightfastness index to be suitable for dyeing wool fabrics for automobile seat covers. The lighter the shade, the greater is the influence of wool yellowing on fastness, the yellowing depending on degradation of the wool due to chemical damage inflicted during the finishing process. Substituting sulfamic acid for H2SO4 for the dye development decreases the damage to the wool fiber and, in some cases, improves lightfastness.
IT **10290-03-6**, Indigosol Brilliant Orange IRK
RL: USES (Uses)
(dyeing of wool fabrics with, for automobile seat covers, lightfastness in)
RN 10290-03-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



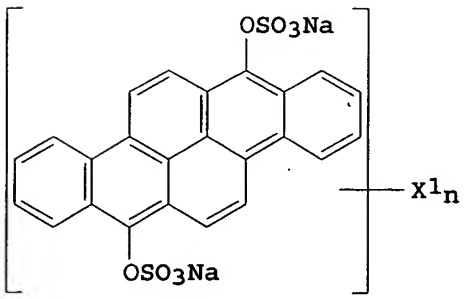
●2 Na

CC 40-6 (Textiles and Fibers)
IT 1324-15-8, Indigosol Golden Yellow IRK 2519-28-0, Indigosol Blue IBC 2538-84-3, Indigosol Green IB 3875-72-7 3956-62-5, Indigosol Yellow V 10126-90-6, Indigosol Red IF2B 10134-35-7 **10290-03-6**, Indigosol Brilliant Orange IRK 12213-66-0, C.I. Solubilised Vat Yellow 45 23594-58-3 23725-15-7, Indigosol Brown IBR 61725-67-5, C.I. Solubilised Vat Black 5
RL: USES (Uses)
(dyeing of wool fabrics with, for automobile seat covers, lightfastness in)

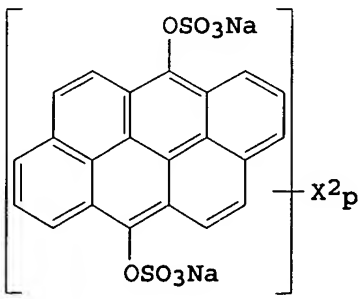
L33 ANSWER 24 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1989:233103 Document No. 110:233103 Orange dye mixtures for dyeing polyester-cotton fiber blends. Gralinski, Miroslaw; Jedrzejewski, Jan; Granat, Krzysztof; Blonska, Wieslawa; Gruszczynski, Tadeusz; Klusek, Eugeniusz; Pekacki, Jerzy (Osrodek Badawczo-Rozwojowy Przemyslu Barwnikow "Organika", Pol.). Pol. PL 132061 B1 19870331, 4 pp. (Polish). CODEN: POXXA7. APPLICATION: PL 1982-235694 19820329.
GI



I



II



III

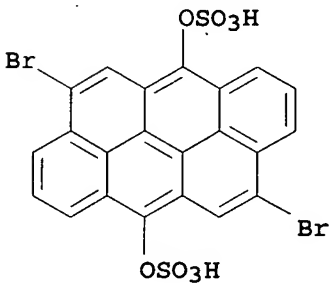
AB An orange dye for polyester-cellulose fiber blends consists of mixts. of I (R1 = H, Me; R2 = H, Cl, Br, CN, MeSO2; X = CmH2m+1

alkyl, CH2CH2OH, AcOCH2CH2; m = 1-4; Y = CH2CH2OH, CH2CH2CN, AcOCH2CH2; Z = NO2) 15-28, II [X1 = H, halogen (especially Br); n = 2-3] 15-24, III [X2 = halogen (especially Cl or Br); p = 2-3] 52-65 parts, and conventional dispersants, lubricants, and wetting agents. A mixture of I (R1 = H, R2 = 2-Cl, X = AcOCH2CH2, Y = CH2CH2CN, Z = 4-NO2) 21.3, II X1 = Br, n = 2) 19.7, and III (X = Br in positions 2 and 8, p = 2) 59 parts was ground and homogenized. The mixture was conventionally applied for uniform dyeing of a 67/33 blend of polyester and cellulosic fibers, producing a fast orange shade.

IT **10290-03-6**
RL: USES (Uses)
(orange dye mixts. containing, for polyester-cellulosic fiber blends)

RN 10290-03-6 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



●2 Na

IC ICM C09B067-00
ICS D06P003-82

CC 40-6 (Textiles and Fibers)
Section cross-reference(s): 41

IT 1324-15-8 6021-61-0 **10290-03-6**
RL: USES (Uses)
(orange dye mixts. containing, for polyester-cellulosic fiber blends)

L33 ANSWER 26 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1985:8139 Document No. 102:8139 Concurrent dyeing and finishing: I - Novel approach to simultaneous dyeing and finishing of PET/cotton blend with one dye class. Ibrahim, N. A.; Hanna, H. L. (Text. Div., Natl. Res. Cent., Cairo, Egypt). American Dyestuff Reporter, 73(10), 36, 38-42, 45-6 (English) 1984. CODEN: ADREAI. ISSN: 0002-8266.

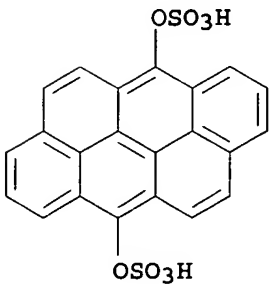
AB The optimum conditions for the title dyeing and finishing process consist of padding the fabric in a solution containing dye 2.5, crosslinking agent based on DMDHEU [1854-26-8] 100, ammonium persulfate 5, oxyethylated antimigrating agent 10, softening agent 3, and wetting agent 2 g/L, drying 5 min at 80°, curing 1 min at 200°, rinsing, development by using H3PO4 and NaNO2, soaping, rinsing, and drying. The process gave ease of application, excellent dye fixation and fastness, reduction in dye and water consumption, good fabric performance, and energy conservation. The soluble vat dyes used were Indigosol Rubine IRB and Indigosol Green.

IT **1324-18-1**
RL: USES (Uses)

(dyeing by, of cotton-polyester blends, with concurrent durable-press finishing)

RN 1324-18-1 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate), disodium salt (7CI, 8CI, 9CI) (CA INDEX NAME)



2 (D1—O—Me)

●2 Na

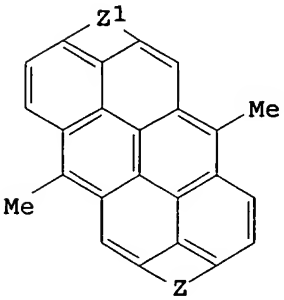
CC 40-6 (Textiles)

IT **1324-18-1** 1324-72-7 12226-70-9
RL: USES (Uses)
(dyeing by, of cotton-polyester blends, with concurrent durable-press finishing)

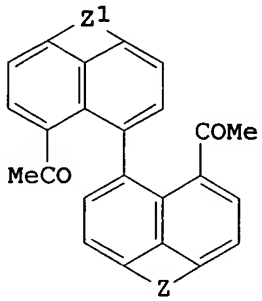
L33 ANSWER 27 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1984:510581 Document No. 101:110581 Derivatives of anthanthrene. Dokunikhin, N. S.; Vorozhtsov, G. N. (USSR). U.S.S.R. SU 283209 A1 19840423 From: Otkrytiya, Izobret., Prom. Obraztsy, Tovarnye Znaki 1984, (15), 233. (Russian). CODEN: URXXAF. APPLICATION: SU 1968-1229956 19680330.

GI



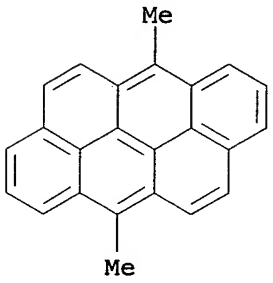
I



II

AB Anthanthrene derivs. [Z, Z1 = CH2XCH2; X = bond, O, (un)substituted NH] were prepared by cyclizing 1,1'-binaphthyl derivs. in the presence of acidic condensing agents, e.g., mixture of POCl3 and concentrated H3PO4.

IT **41217-05-4DP**, cyclic derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by cyclocondensation reaction of diacetylbinaphthyl derivs.)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)

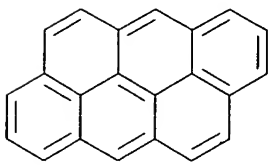


IC C07C015-28
CC 25-28 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
IT **41217-05-4DP**, cyclic derivs.
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, by cyclocondensation reaction of diacetylbinaphthyl derivs.)

L33 ANSWER 28 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1984:211751 Document No. 100:211751 Forming thin organic films. (Futaba Denshi Kogyo Co., Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 58167602 A2 19831003 Showa, 10 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1982-49174 19820329.
AB An organic material, e.g. anthracene or anthanthrene, is heated in a crucible, and the vapor formed is discharged via a jet nozzle into a vacuum to form a supercooled cluster beam by adiabatic expansion during the ejection. If necessary, the beam is ionized and accelerated or decelerated and guided to a target substrate to form a thin film by condensation or polymerization having excellent adhesion to the substrate.
IT **90386-01-9**
RL: TEM (Technical or engineered material use); USES (Uses)
(coatings, vapor cluster beam in application of)
RN 90386-01-9 HCAPLUS
CN Dibenzo[def,mno]chrysene, homopolymer (9CI) (CA INDEX NAME)

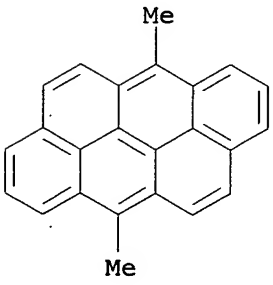
CM 1

CRN 191-26-4
CMF C22 H12

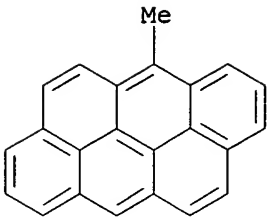


IC C08F002-52
CC 42-2 (Coatings, Inks, and Related Products)
IT 25135-15-3 **90386-01-9**
RL: TEM (Technical or engineered material use); USES (Uses)
(coatings, vapor cluster beam in application of)

L33 ANSWER 29 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1984:116200 Document No. 100:116200 The relationship between ionization potential and horseradish peroxidase/hydrogen peroxide-catalyzed binding of aromatic hydrocarbons to DNA. Cavalieri, Ercole L.; Rogan, Eleanor G.; Roth, Robert W.; Saugier, Richard K.; Hakam, Alaeddin (Med. Cent., Univ. Nebraska, Omaha, NE, 68105, USA). Chemico-Biological Interactions, 47(1), 87-109 (English) 1983. CODEN: CBINA8. ISSN: 0009-2797.
AB The ionization potentials (IP) of 91 alternant polycyclic aromatic hydrocarbons (PAH) were determined from the absorption maximum of the charge-transfer complex of each hydrocarbon and chloranil in CHCl3. The extent of horseradish peroxidase [9003-99-0] (HRP)-catalyzed binding to DNA of 14 hydrocarbons of varying IP was measured. Only hydrocarbons with IP < approx. 7.35 eV were significantly bound to DNA. These results provide further evidence that HRP-mediated binding of PAH to DNA occurs by 1-electron oxidation and indicate that hydrocarbons must have IP < approx. 7.35 eV to be activated by 1-electron oxidation Thus, determination of IP and HRP-catalyzed binding to DNA can offer some guidelines for selecting aromatic hydrocarbons which might undergo carcinogenic activation by this mechanism.
IT **41217-05-4**
RL: BIOL (Biological study)
(horseradish peroxidase activated binding of, to DNA, carcinogenicity and ionization potential in relation to)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)

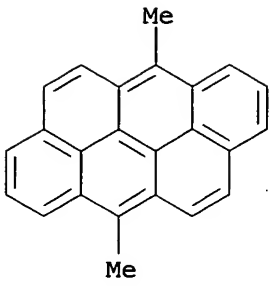


IT **31927-64-7**
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(ionization potential of, carcinogenicity in relation to)
RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



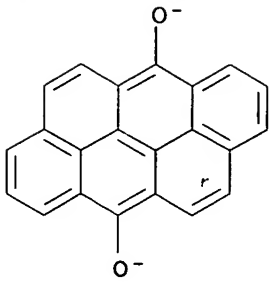
CC 4-6 (Toxicology)
IT 50-32-8, biological studies 53-70-3 56-49-5 56-55-3 57-97-6
85-01-8, biological studies 120-12-7, biological studies
129-00-0, biological studies 191-26-4 192-97-2 2381-39-7
2541-69-7 3697-24-3 **41217-05-4**
RL: BIOL (Biological study)
(horseradish peroxidase activated binding of, to DNA, carcinogenicity and ionization potential in relation to)
IT 71-43-2, properties 91-20-3, properties 92-24-0 189-55-9
189-64-0 191-07-1 191-24-2 191-30-0 192-47-2 192-51-8
192-65-4 195-19-7 198-55-0 213-46-7 215-58-7 217-59-4
218-01-9 224-41-9 316-14-3 317-64-6 568-81-0 652-04-0
781-43-1 1705-85-7 2319-96-2 2381-16-0 2381-19-3 2381-21-7
2381-31-9 2381-34-2 2422-79-9 2498-75-1 2498-76-2
2498-77-3 2606-85-1 3353-12-6 3442-78-2 3697-30-1
4076-39-5 4076-40-8 4514-19-6 6111-78-0 16757-80-5
16757-81-6 16757-82-7 16757-83-8 16757-84-9 16757-85-0
16757-86-1 16757-87-2 16757-88-3 16757-89-4 16757-90-7
16757-91-8 18868-66-1 20627-34-3 21248-00-0 25732-74-5
31647-36-6 **31927-64-7** 39000-82-3 40568-90-9
59417-86-6 61735-77-1 61735-78-2 63041-61-2 63041-62-3
63041-76-9 63041-77-0 63104-32-5 63104-33-6 70644-19-8
73368-38-4 74924-89-3 74924-90-6 78694-66-3 82721-25-3
RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)
(ionization potential of, carcinogenicity in relation to)

L33 ANSWER 30 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1984:85035 Document No. 100:85035 Reactivity of PAH [polycyclic aromatic hydrocarbons] in UV- and γ-radiation initiated oxidation reactions. Paalme, L.; Uibopuu, H.; Rohtla, I.; Pahapill, J.; Gubergrits, M.; Jacquignon, Pierre C. (Inst. Chem., Tallinn, USSR). Polynucl. Aromat. Hydrocarbons, Int. Symp., 7th, Meeting Date 1982, 999-1008. Editor(s): Cooke, Marcus; Dennis, Anthony J. Battelle Press: Columbus, Ohio. (English) 1983. CODEN: 50NNAZ.
AB The kinetics of the title reaction of 70 PAH were determined The reactivity of PAH in initiated oxidation in organic solvents correlated with both the value of the free valency of the most active C atom and the localization energy of its bonds. Good correlations were also obtained with excited-state energies. In aqueous solns., the oxidation probably occurs via a triplet-state radical mechanism. The correlation equations were valid only for groups of compds., e.g., nonalternant and alternant or N-containing PAH.
IT **41217-05-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(UV- or γ-radiation initiated oxidation of, kinetics of)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



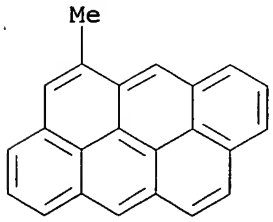
CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 1
IT 50-32-8, reactions 53-70-3 56-49-5 56-55-3 57-97-6
71-43-2, reactions 83-32-9 85-01-8, reactions 86-73-7
86-74-8 91-20-3, reactions 92-24-0 92-82-0 120-12-7,
reactions 129-00-0, reactions 189-55-9 189-64-0 191-07-1
191-24-2 191-26-4 191-30-0 192-47-2 192-51-8 192-65-4
192-97-2 194-59-2 198-55-0 203-07-6 203-20-3 205-99-2
206-06-4 206-44-0 207-08-9 207-84-1 215-58-7 217-59-4
218-01-9 224-41-9 224-42-0 224-53-3 225-11-6 225-51-4
226-36-8 239-64-5 260-94-6 2381-39-7 2422-79-9 2498-75-1
2541-69-7 4217-52-1 5385-75-1 16757-84-9 16757-90-7
16757-91-8 27093-62-5 36762-03-5 36762-07-9 36762-09-1
40568-90-9 **41217-05-4** 59968-92-2 88778-42-1
88778-43-2 88778-44-3 88778-45-4 88778-46-5 88778-47-6
88778-48-7 88778-49-8 88778-50-1
RL: RCT (Reactant); RACT (Reactant or reagent)
(UV- or γ-radiation initiated oxidation of, kinetics of)

L33 ANSWER 31 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1984:76086 Document No. 100:76086 Ion-pairing between anthanthrone anions and divalent metal cations and adsorption of ion-pairs on mercury electrodes in N,N-dimethylformamide. Nagaoka, Tsutomu; Okazaki, Satoshi (Fac. Sci., Kyoto Univ., Kyoto, 606, Japan). Journal of Electroanalytical Chemistry and Interfacial Electrochemistry, 158(1), 139-51 (English) 1983. CODEN: JEIEBC. ISSN: 0022-0728.
AB The electrochem. behavior of ion-pairs of anthanthrone anions was examined and it was found that the ion-pairs were adsorbed by Hg electrodes in the presence of divalent metal ions. The mechanism of ion-pair adsorption is discussed as well as that of ion-pairing in solution Since the ion-pairs were not adsorbed on Au electrodes, specific interaction between surface Hg atoms and the anthanthrone anion was present, even at the neg. charged surface. The possible structure and orientation of the ion-pairs at the surface are discussed.
IT **88850-02-6**
RL: PRP (Properties)
(ion pairing with divalent metal ions, adsorption of pairs by mercury electrode in DMF in relation to)
RN 88850-02-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, ion(2-) (9CI) (CA INDEX NAME)



CC 72-2 (Electrochemistry)
Section cross-reference(s): 22, 66
IT 72645-64-8 **88850-02-6**
RL: PRP (Properties)
(ion pairing with divalent metal ions, adsorption of pairs by mercury electrode in DMF in relation to)

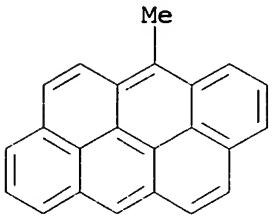
L33 ANSWER 32 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1983:452628 Document No. 99:52628 Quantitative sequence of the conjugative effect of even benzenoid hydrocarbons. Li, Sen (Tongji Univ., Shanghai, Peop. Rep. China). Tongji Daxue Xuebao, Ziran Kexueban (4), 11-17 (Chinese) 1982. CODEN: TTHPDJ. ISSN: 0253-374X.
AB The decrease (q) in charge densities on Me groups attached to even benzenoid hydrocarbons were determined Values of (1-q) were correlated with conjugative effects of the benzenoid arenes. Values of (1 - q) were also correlated with Chiang's factor for homologous series. For electron affinity, polarog. reductive and/or oxidative half-wave potentials, resonance energies per electron, and ionization potentials, etc., the solving linear relationship was observed: P = A(1 - q) + B (P = structural parameter; A, B = consts.). Also, values of (1 - q) were correlated with σr (aryl group substituent parameters).
IT **83321-50-0**
RL: USES (Uses)
(charge d. delocalization in)
RN 83321-50-0 HCAPLUS
CN Dibenzo[def,mno]chrysene, 5-methyl- (9CI) (CA INDEX NAME)



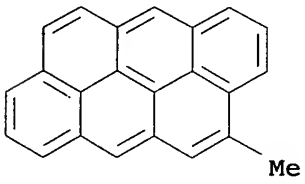
CC 22-2 (Physical Organic Chemistry)
IT 71-43-2, uses and miscellaneous 90-12-0 217-59-4 644-08-6
652-04-0 883-20-5 1523-23-5 1705-85-7 2381-31-9 3353-12-6
7499-40-3 10350-33-1 13119-86-3 17278-93-2 19224-38-5
63041-77-0 80251-99-6 **83321-50-0** 86476-81-5
86476-82-6 86476-83-7 86476-84-8 86476-85-9 86476-86-0
86476-87-1 86476-88-2 86476-89-3 86476-90-6 86476-91-7

86476-92-8 86476-93-9 86476-94-0 86476-95-1 86476-96-2
86476-97-3 86482-31-7 86482-32-8
RL: USES (Uses)
(charge d. delocalization in)

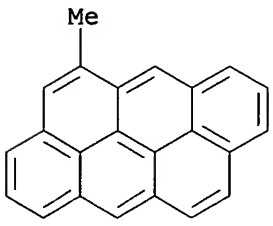
L33 ANSWER 33 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1982:562211 Document No. 97:162211 Calculation of chemical shifts of condensed aromatic hydrocarbon series. II. Additivity in the methyl proton chemical shifts of methylated condensed aromatic hydrocarbons. Cao, Huaizhen; Liu, Chunwan (Fujian Inst. Res. Struct. Matter, Acad. Sinica, Fuzhou, Peop. Rep. China). Huaxue Xuebao, 40(6), 481-7 (Chinese) 1982. CODEN: HHHPA4. ISSN: 0567-7351.
AB Calculated Me proton chemical shifts of methylated condensed aromatic hydrocarbons agree with exptl. values. The standard error is 0.99 ppm.
IT **31927-64-7 83321-49-7 83321-50-0**
RL: PRP (Properties)
(Me group NMR chemical shifts in, calcn. of)
RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 83321-49-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 4-methyl- (9CI) (CA INDEX NAME)



RN 83321-50-0 HCAPLUS
CN Dibenzo[def,mno]chrysene, 5-methyl- (9CI) (CA INDEX NAME)



CC 22-10 (Physical Organic Chemistry)

IT 90-12-0 91-57-6 108-88-3, properties 316-49-4 610-48-0
613-12-7 652-04-0 779-02-2 832-64-4 832-69-9 832-71-3
883-20-5 1705-84-6 1705-85-7 2319-96-2 2381-15-9 2381-16-0
2381-21-7 2381-34-2 2531-84-2 2606-85-1 2869-60-5
2871-91-2 3353-12-6 3442-78-2 3697-24-3 4076-40-8
5950-66-3 5950-67-4 10329-20-1 10350-33-1 13119-86-3
13322-53-7 14214-56-3 15299-16-8 19224-38-5 19224-40-9
24471-47-4 **31927-64-7** 33942-87-9 58706-01-7
63041-95-2 66374-87-6 66778-25-4 78377-41-0 78377-42-1
80251-98-5 80251-99-6 80252-00-2 80252-01-3 83321-33-9
83321-34-0 83321-35-1 83321-36-2 83321-37-3 83321-38-4
83321-39-5 83321-40-8 83321-41-9 83321-42-0 83321-43-1
83321-44-2 83321-45-3 83321-46-4 83321-47-5 83321-48-6
83321-49-7 **83321-50-0** 83321-51-1 83321-52-2
83321-53-3 83321-54-4 83321-55-5 83321-56-6 83321-57-7
83321-58-8 83321-59-9 83321-60-2 83321-61-3 83321-62-4
83321-63-5 83321-64-6 83321-65-7 83321-66-8 83321-67-9
83321-68-0 83321-69-1 83321-70-4 83321-71-5 83321-72-6
83321-73-7 83321-74-8 83321-75-9 83321-76-0 83321-77-1
83321-78-2 83321-79-3 83321-80-6 83321-81-7 83321-82-8
83321-83-9 83321-84-0 83321-85-1 83321-86-2 83321-87-3
83321-88-4 83321-89-5 83321-90-8 83321-91-9 83321-92-0
83321-93-1 83334-71-8
RL: PRP (Properties)
(Me group NMR chemical shifts in, calcn. of)

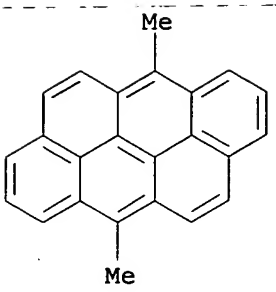
L33 ANSWER 34 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1982:405606 Document No. 97:5606 Reactivity of dibenzopyrenes in UV- and γ-radiation initiated oxidation reactions. Paalme, L.; Uibopuu, H.; Pahapill, J.; Gubergrits, M.; Bahna, L.; Jacquignon, P. C. (Inst. Chem., Tallinn, USSR). Neoplasma, 29(1), 29-35 (English) 1982. CODEN: NEOLA4. ISSN: 0028-2685.

AB Kinetics of UV- and γ-irradiation-initiated oxidative degradation of dibenzopyrenes, for example, benzo[a]pyrene, anthanthrene, were determined The apparent 0-order reaction gave mainly the corresponding quinones. The relative rate consts. for both reactions (photochem. and radiolytic oxidation) were correlated, except in the case of the highly carcinogenic compound 1,2,3,4-dibenzopyrene, which exhibits extremely high reactivity during photoinduced oxidation Relative reactivities of dibenzopyrenes towards photoinitiated oxidation exponentially decreased with increasing lowest singlet and triplet excited state energies. Also, the relative rate consts. were correlated with data for polarog. reduction This correlation was not found in the case of radiolytic oxidation

IT **41217-05-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(UV- and γ-irradiation-initiated oxidation of, kinetics of)

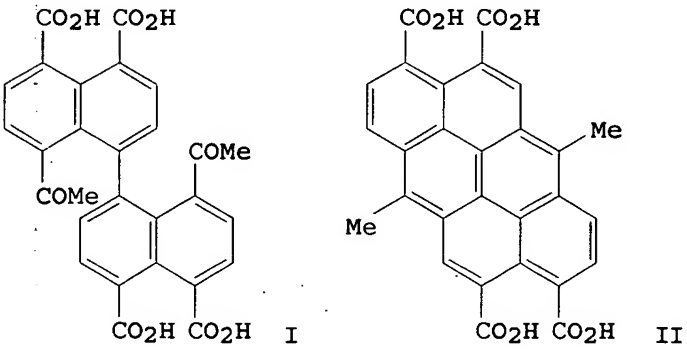
RN 41217-05-4 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)

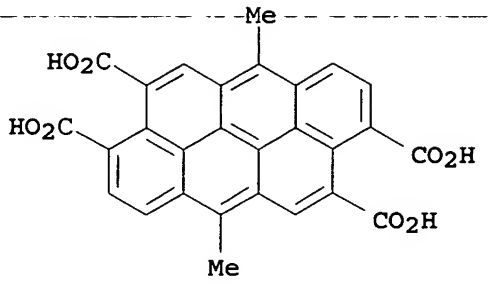


CC 22-7 (Physical Organic Chemistry)
IT 50-32-8, reactions 189-55-9 189-64-0 191-26-4 191-30-0 192-47-2 192-51-8 192-65-4 **41217-05-4**
RL: RCT (Reactant); RACT (Reactant or reagent)
(UV- and γ-irradiation-initiated oxidation of, kinetics of)

L33 ANSWER 35 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1981:496614 Document No. 95:96614 Electrochemical study of the cyclization of 1,1'-binaphthyl derivatives. IV. Polarographic reduction and cyclization of 1,1'-binaphthyl-4,4',5,5'-tetracarboxylic acid derivatives. Khmel'nitskaya, E. Yu.; Romanova, K. A.; Vorozhtsov, G. N. (Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR). Zhurnal Obshchei Khimii, 51(5), 1187-93 (Russian) 1981. CODEN: ZOKHA4. ISSN: 0044-460X.
GI

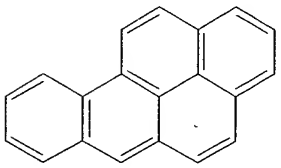


AB The electrochem. reduction of I gave II, but the analogous treatment of the dianhydride of I gave only 12-5% cyclized product and no cyclization was observed with the N,N'-diphenyl diimide or the tetra-Me ester. Polarog. data indicated that large substituents in the 8 and 8' positions of 1,1'-binaphthyl prevent conjugation between the naphthalene rings; only the inductive effect is retained.
IT **54481-18-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. cyclization of binaphthalenetetracarboxylic acid derivs.)
RN 54481-18-4 HCAPLUS
CN Dibenzo[def,mno]chrysene-3,4,9,10-tetracarboxylic acid, 6,12-dimethyl- (9CI) (CA INDEX NAME)



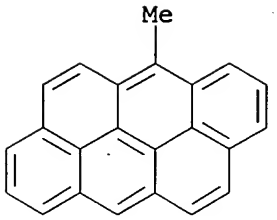
CC 22-5 (Physical Organic Chemistry)
Section cross-reference(s): 72
IT **54481-18-4P**
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, in electrochem. cyclization of binaphthalenetetracarboxylic acid derivs.)

L33 ANSWER 36 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1981:475128 Document No. 95:75128 Rat mammary gland versus mouse skin: different mechanisms of activation of aromatic hydrocarbons.
Cavalieri, E.; Sinha, D.; Rogan, E. (Med. Cent., Univ. Nebraska, Omaha, NE, 68105, USA). Polynucl. Aromat. Hydrocarbons: Chem. Biol. Eff., Int. Symp., 4th, Meeting Date 1979, 215-31. Editor(s): Bjoerseth, Alf; Dennis, Anthony J. Battelle Press: Columbus, Ohio. (English) 1980. CODEN: 45WTAI.
GI

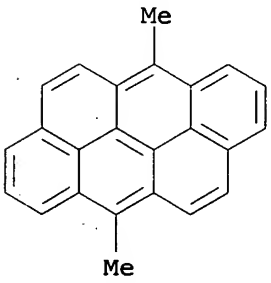


I

AB The carcinogenic effect of a series of polycyclic aromatic hydrocarbons (PAHs) having different ionization potentials on mammary gland was compared with that on the mouse skin to examine the postulation that the mammary gland might activate PAHs selectively by 1-electron oxidation Mammary tumors were inducted by the direct application of PAHs. The mammary tumor incidence with benzo[a]pyrene (I) [50-32-8] and 7,12-dimethylbenz[a]anthracene [57-97-6] were 80 and 100%, resp. The tumor-initiating activity of I and benzo[a]pyrene 7,8-dihydrodiol [13345-25-0] on mouse skin was about the same when applied in Me2CO, whereas in rat mammary gland, only I was active. Compds. like 5-methylchrysene [3697-24-3] and dibenz[a,h]anthracene [53-70-3], which have relatively high ionization potential and thus cannot be activated by 1-electron oxidation, are inactive in the mammary gland, but are potent carcinogens on mouse skin.
IT **31927-64-7 41217-05-4**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenicity of, of skin)
RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



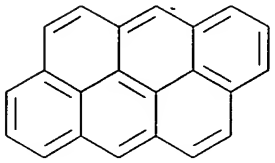
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-7 (Toxicology)
IT 56-49-5 120-12-7, biological studies **31927-64-7**
41217-05-4
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(carcinogenicity of, of skin)

L33 ANSWER 37 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1981:177606 Document No. 94:177606 Preliminary lipid analyses of Sections 440A-7-6, 440B-3-5, 440B-8-4, 440B-68-2, and 436-11-4: Legs 56 and 57, Deep Sea Drilling Project. Brassell, S. C.; Comet, P. A.; Eglinton, G.; Isaacson, P. J.; McEvoy, J.; Maxwell, J. R.; Thomson, I. D.; Tibbetts, P. J. C.; Volkman, J. K.; et al. (Sch. Chem., Univ. Bristol, Bristol, BS8 1TS, UK). Initial Rep. Deep Sea Drill. Proj., Volume 56-57, Issue 2, 1367-90. GPO: Washington, D. C. (English) 1980. CODEN: 22OIA4.
AB Bound and free solvent-extractable lipids from the title sections were examined The compound classes studied include aliphatic and aromatic hydrocarbons, ketones, alcs., and carboxylic acids. Carotenoids and humic acids were also examined The quant. results are considered in terms of input indicators, diagenesis parameters, and structural classes. A difference in input is deduced across the Japan Trench, with a higher proportion of autochthonous components on the western inner trench slope than on the outer, and greater input in the early Pleistocene than in the Miocene. A variety of diagenetic transformations is observed at Site 440 as sample depth increases. The results are compared with those of samples from Atlantic Cretaceous sediments and from the Walvis Bay area.
IT **41699-10-9**
RL: OCCU (Occurrence)
(in sedimentary rocks, geochem. in relation to, of Japan Trench)

RN 41699-10-9 HCAPLUS
CN Dibenzo[def,mno]chrysene, methyl- (9CI) (CA INDEX NAME)



D1—Me

CC 51-1 (Fossil Fuels, Derivatives, and Related Products)
Section cross-reference(s): 53

IT 57-10-3, occurrence 57-11-4, occurrence 57-88-5, occurrence
80-97-7 85-01-8, occurrence 85-01-8D, C<3 alkyl derivs.
111-01-3 111-20-6, occurrence 112-42-5 112-53-8 112-70-9
112-72-1 112-85-6 112-92-5 112-95-8 123-99-9, occurrence
129-00-0, occurrence 129-00-0D, C<3 alkyl derivs. 143-07-7,
occurrence 150-86-7 191-07-1 191-24-2 191-26-4 192-97-2
193-39-5 198-55-0 198-55-0D, C<3 alkyl derivs. 205-82-3
206-44-0 206-44-0D, C<3 alkyl derivs. 218-01-9 218-01-9D, C<3
alkyl derivs. 360-68-9 471-62-5 474-63-5 481-21-0 483-65-8
505-52-2 505-54-4 505-55-5 505-56-6 505-95-3 506-12-7
506-13-8 506-30-9 506-38-7 506-46-7 506-48-9 506-50-3
506-51-4 506-52-5 508-09-8 514-07-8 544-63-8, occurrence
544-76-3 544-85-4 546-99-6 557-59-5 557-61-9 559-74-0
593-45-3 593-49-7 593-50-0 629-62-9 629-66-3 629-76-5
629-78-7 629-92-5 629-94-7 629-96-9 629-97-0 629-99-2
630-01-3 630-02-4 630-03-5 630-04-6 630-05-7 630-07-9
638-36-8 638-53-9 638-67-5 638-68-6 638-96-0 638-97-1
646-30-0 646-31-1 661-19-8 693-23-2 747-90-0 764-67-0
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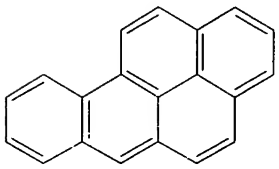
1454-84-8 1454-85-9 1460-18-0 1615-91-4 1615-92-5
1852-04-6 1883-13-2 1921-70-6 1961-72-4 2004-39-9
2345-28-0 2363-71-5 2398-34-7 2424-90-0 2424-92-2
2433-96-7 2450-31-9 2638-57-5 2734-37-4 2922-51-2
3133-01-5 3258-87-5 3365-67-1 3625-52-3 4250-38-8
4552-17-4 4617-33-8 4970-37-0 5632-97-3 5638-06-2
6250-70-0 6624-76-6 7138-40-1 7235-40-7 7320-54-9
7373-13-9 7735-38-8 7796-19-2 10379-52-9 13099-34-8
13849-96-2 14167-59-0 14292-26-3 15594-90-8 15896-36-3
15910-23-3 17105-72-5 17278-74-9 17600-99-6 17773-30-7
18472-36-1 18787-63-8 19044-02-1 19044-06-5 21681-17-4
22438-61-5 22589-04-4 23929-42-2 26040-98-2 26636-62-4
26764-25-0 27530-79-6 27577-90-8 29703-52-4 30997-39-8
31063-73-7 31469-30-4 31711-53-2 32602-69-0 32602-70-3
34347-28-9 36653-82-4 36728-72-0 38232-01-8 38788-81-7
38885-94-8 39832-31-0 40165-89-7 41637-90-5 41699-09-6
41699-10-9 50313-71-8 51271-94-4 52655-09-1
53282-68-1 53584-61-5 53584-62-6 54311-28-3 54311-31-8
55066-73-4 56362-45-9 58524-92-8 58560-37-5 58560-38-6
59905-70-3 60208-82-4 62123-19-7 62643-46-3 64031-91-0
64158-98-1 65132-06-1 65754-98-5 65754-99-6 65755-17-1
66988-08-7 67069-21-0 67069-24-3 67882-24-0 68947-37-5
69088-88-6 69256-43-5 69521-46-6 69760-74-3 69760-76-5

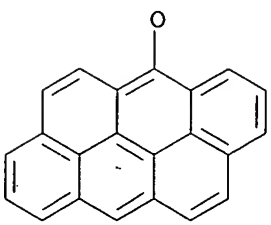
69780-28-5 69977-26-0 72778-32-6 72778-33-7 72778-34-8
73292-33-8 73292-42-9 73292-43-0 73303-36-3 74229-82-6
74229-83-7 75207-54-4 75207-55-5 75207-57-7 77194-04-8
77194-05-9 77194-07-1 77194-08-2 77194-10-6 77194-11-7
77194-13-9 77194-14-0 77298-86-3 77306-97-9 77306-99-1
77307-01-8 77307-02-9 77307-03-0 77307-06-3
RL: OCCU (Occurrence)
(in sedimentary rocks, geochem. in relation to, of Japan Trench).

L33 ANSWER 38 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1980:70742 Document No. 92:70742 Metabolic activation of chemical carcinogens and binding of metabolites with nucleic acid bases. Nagata, Chikayoshi; Kodama, Masahiko; Kimura, Teruyuki; Yamaguchi, Tamie (Biophys. Div., Natl. Cancer Cent. Res. Inst., Tokyo, 104, Japan). International Journal of Quantum Chemistry, 16(4), 917-30 (English) 1979. CODEN: IJQCB2. ISSN: 0020-7608.
GI



I

AB A free radical was produced enzymically by incubation benzo[a]pyrene (I) [50-32-8] with liver microsomes. This 6-oxybenzo[a]pyrene radical [20928-82-9] was sufficiently reactive to bind covalently with nucleic acid bases. Similar reactive free radicals were produced enzymically from anthanthrene [191-26-4] and 10-azabenzo[a]pyrene [189-92-4], which were carcinogenic in spite of lacking the bay regions. 3'-Methyl-4-dimethylaminoazobenzene [55-80-1] and naphthylamines, and 2-acetylaminofluorene [70377-63-8] yielded free radicals after incubation with liver microsomes. Thus, various chemical carcinogens can be converted to free radicals suggesting causal significance for the formation of free radicals in chemical carcinogenesis.
IT **72616-34-3**
RL: BIOL (Biological study)
(nucleic acid binding response to, carcinogenesis in relation to)
RN 72616-34-3 HCAPLUS
CN Dibenzo[def,mno]chrysen-6-yloxy (9CI) (CA INDEX NAME)



CC 4-7 (Toxicology)
IT 16518-49-3 69285-93-4 **72616-34-3** 72616-35-4
72616-36-5 72616-37-6 72616-38-7 72616-39-8 72616-40-1

72645-64-8
RL: BIOL (Biological study)
(nucleic acid binding response to, carcinogenesis in relation to)

L33 ANSWER 39 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1979:585313 Document No. 91:185313 Electrical properties and constitution of several low-resistivity iodine complexes. Doi, Susumu; Fujita, Akiyoshi; Ikeura, Shigeo; Inabe, Tamotsu; Matsunaga, Yoshio (Fac. Sci., Hokkaido Univ., Sapporo, 060, Japan). Bulletin of the Chemical Society of Japan, 52(9), 2494-500 (English) 1979. CODEN: BCSJA8. ISSN: 0009-2673.

AB The elec. resistivity and Seebeck coefficient of the I complexes with 8 aromatic compds. were examined as functions of the composition and the temperature The formation of complexes is indicated by maximum or shoulders in the resistivity-composition isotherms at the following compns.: (anthanthrene)2I9, (6,12-dioxoanthanthrene)I2, (6,12-dioxoanthanthrene)I3, (pyranthrene)I3, (violanthrene)2I7, (phthalocyanine)I2, (phthalocyanine)I5, (phenoxazine)2I3, (pyridazine)5I9, and (N,N'-diphenyl-p-phenylenediamine)5I13. Furthermore, some sharp resistivity min. are considered as evidence of the complex formation: e.g., (6,12-dioxoanthanthrene)2I3 and (phthalocyanine)2I3. On the basis of these compns., a nonintegral formal oxidation state for the organic mols. and the presence of iodine as triiodide or higher polyiodide ions are established for most of the complexes.

IT **71815-67-3**
RL: PRP (Properties)
(elec. resistance and thermoelectricity of)

RN 71815-67-3 HCAPLUS

CN Dibenzo[def,mno]chrysene, compd. with iodine (4:9) (9CI) (CA INDEX NAME)

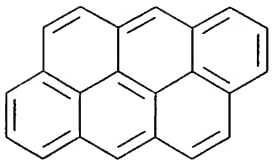
CM 1

CRN 7553-56-2
CMF I2

I—I

CM 2

CRN 191-26-4
CMF C22 H12



CC 76-2 (Electric Phenomena)

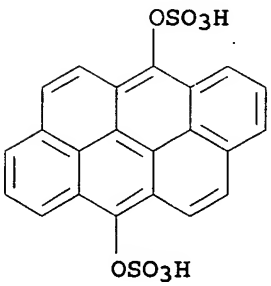
IT 7553-56-2D, aromatic complexes 66582-63-6 **71815-67-3**
71815-68-4 71815-69-5 71815-70-8 71815-71-9 71815-72-0
71815-73-1 71815-74-2 71815-75-3

RL: PRP (Properties)
(elec. resistance and thermoelectricity of)

L33 ANSWER 40 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1979:214577 Document No. 90:214577 Anthraquinone dyes as new reagents in chemical analysis. Gregorowicz, Zbigniew; Kowalski, Stanislaw; Gorka, Piotr (Inst. Chem. Anal. Ogol. Politech. Slaskiej Gliwicach, Gliwice, Pol.). Przemysl Chemiczny, 57(12), 636-8 (Polish) 1978. CODEN: PRCHAB. ISSN: 0033-2496.

AB Some spectrophotometric, chromatog., derivatog. and potentiometric studies were conducted on 2 synthetic anthraquinone derivative dyes, Helasol Green 2G (I) (C.I. 59831, Solubilized Vat Green 2), and Helasol Violet 4R (II) (C.I. 59321, Solubilized Vat Violet 7). The dyes exhibit redox properties. To obtain sufficient reagent from the tech. dye, 5 cm3 acetate buffer (pH 2) and 5 cm3 0.1% aqueous I solution were mixed and extracted with 10 cm3 3:1 CHCl3-EtOH within 1 min. The organic phase was rejected and the dye left in the aqueous phase was used to determine Fe(III) and Cr(VI). The refining procedure was similar for both dyes: for II, 3 cm3 buffer and 10 cm3 1:1 CHCl3-EtOH were used. Dyes coming from different technol. lots were equally useful for anal. purposes despite differences in their composition The use of the dyes as reagents in spectrophotometry, potentiometry, and paper chromatog. is discussed.

IT **1324-23-8**
RL: ANST (Analytical study)
(as anal. reagent)
RN 1324-23-8 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, diethoxy-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



2 (D1—O—Et)

●2 Na

CC 79-3 (Inorganic Analytical Chemistry)
IT **1324-23-8** 1324-72-7
RL: ANST (Analytical study)
(as anal. reagent)

L33 ANSWER 41 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1979:145314 Document No. 90:145314 Spectrophotometric determination of iron(III) and chromium(VI) using Helasol Violet 4R. Gregorowicz,

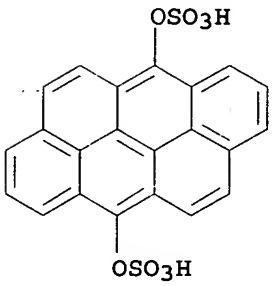
Z.; Gorka, P.; Kowalski, St. (Inst. Anal. Chem., Schlesischen Tech. Hochsch., Gliwice, Pol.). Fresenius' Zeitschrift fuer Analytische Chemie, 294(4), 285 (German) 1979. CODEN: ZACFAU. ISSN: 0016-1152.

AB Prior to the determination, Helasol Violet 4R was purified from its oxidized form by extraction from pH 2 acetate buffer solution with 1:1 CHCl3-EtOH. The organic phase was discarded and the sample solution was added to the reagent solution (where the reagent is stoichiometrically oxidized). CHCl3 was added to 10 mL and the absorbance was measured at 580 nm. The molar absorptivities were 1.9600 + 104 and 2.0800 + 104 for Fe and Cr, resp. Alkalies, Al, Pb, Zn, Ag, SO42-, NO3-, Cl-, CO32-, and PO43- (1000-fold excess) do not interfere. Cu(II), Hg(II), and Pt-group metals interfere. Cu can be masked with NH4Cl.

IT **1324-23-8**
RL: ANST (Analytical study)
(in determination of chromium and iron by spectrophotometry)

RN 1324-23-8 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, diethoxy-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)



2 (D1--O--Et)

●2 Na

CC 79-6 (Inorganic Analytical Chemistry)

IT **1324-23-8**
RL: ANST (Analytical study)
(in determination of chromium and iron by spectrophotometry)

L33 ANSWER 42 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

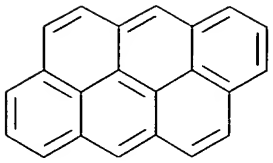
1979:71487 Document No. 90:71487 Kinetics of the photoinitiated oxidation of benzo derivatives of pyrene. Paalme, L.; Gubergrits, M.; Perin, Francois; Jacquignon, Pierre (USSR). Okislenie Kantserogen. Politsiklich. Uglevodorodov Proizvodnykh Benz(a)Pirena 34-43 From: Ref. Zh., Khim. 1978, Abstr. No. 20B1230 (Russian) 1978.

AB Title only translated.

IT **64760-24-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photoinitiated oxidation of, kinetics of)

RN 64760-24-3 HCAPLUS

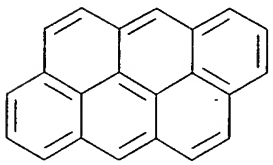
CN Dibenzo[def,mno]chrysene, dimethyl- (9CI) (CA INDEX NAME)



2 (D1—Me)

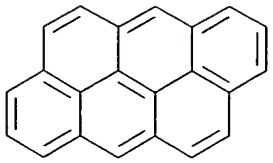
CC 22-5 (Physical Organic Chemistry)
IT 50-32-8, reactions 189-55-9 189-64-0 191-26-4 191-30-0
192-47-2 192-51-8 192-65-4 **64760-24-3**
RL: RCT (Reactant); RACT (Reactant or reagent)
(photoinitiated oxidation of, kinetics of)

L33 ANSWER 43 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:580949 Document No. 87:180949 The identification of high molecular weight polynuclear aromatic hydrocarbons in a biologically active fraction of cigarette smoke condensate. Snook, M. E.; Severson, R. F.; Arrendale, R. F.; Higman, H. C.; Chortyk, O. T. (Tob. Lab., ARS, Athens, GA, USA). Beitraege zur Tabakforschung, 9(2), 79-101 (English) 1977. CODEN: BETAAY. ISSN: 0005-819X.
AB A gel filtration chromatog. method was developed for the isolation and concentration of the high-mol.-weight polynuclear aromatic hydrocarbons (PAH) contained in the most biol. active fraction of cigarette smoke condensate (CSC). The unusually complex mixture of large PAH found in CSC necessitated the use of preparative gas chromatog. followed by high-pressure liquid chromatog. to achieve separation and identifiction. Mass spectral, UV absorption, and chromatog. retention data were needed for the comprehensive identification of the large-mol.-weight PAH components of CSC. The majority of the 200 isolated compds. were identified. Compds. newly identified in CSC included 3,4-dimethylenepyrene, 3,4-trimethylenepyrene, cyclopenta(c,d)pyrene, 4,5-methylenetriphenylene, benzo(b)perylene, and several dibenzofluoranthenes.
IT **41699-10-9 64760-24-3**
RL: BIOL (Biological study)
(in cigarette smoke condensate)
RN 41699-10-9 HCAPLUS
CN Dibenzo[def,mno]chrysene, methyl- (9CI) (CA INDEX NAME)



D1—Me

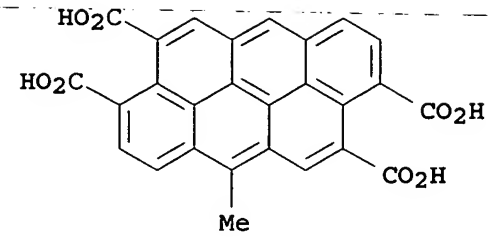
RN 64760-24-3 HCAPLUS
CN Dibenzo[def,mno]chrysene, dimethyl- (9CI) (CA INDEX NAME)



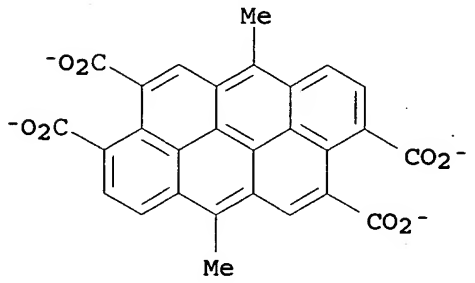
2 (D1—Me)

CC 11-7 (Plant Biochemistry)
IT 50-32-8, biological studies 53-70-3 56-55-3 129-00-0, biological studies 189-64-0 191-07-1 191-24-2 191-26-4 191-30-0 192-51-8 192-65-4 192-97-2 193-39-5 193-43-1 195-19-7 197-70-6 198-55-0 201-06-9 202-98-2 203-12-3 203-33-8 203-64-5 205-12-9 205-82-3 205-99-2 206-44-0 207-08-9 213-46-7 215-58-7 217-59-4 218-01-9 224-41-9 243-17-4 1705-85-7 2381-21-7 3351-28-8 3351-31-3 3351-32-4 3353-12-6 3442-78-2 5385-22-8 5385-75-1 7130-15-6 13119-86-3 20485-57-8 23992-32-7 25167-89-9 25732-74-5 25889-60-5 27208-37-3 29062-98-4 30582-03-7 33543-31-6 41637-89-2 41637-92-7 41637-94-9 41699-04-1 41699-06-3 41699-09-6 **41699-10-9** 43178-07-0 43178-22-9 51001-44-6 60382-88-9 60826-65-5 60826-67-7 60826-74-6 60826-75-7 60826-76-8 64031-91-0 64158-98-1 64158-99-2 64760-14-1 64760-15-2 64760-18-5 64760-19-6 64760-20-9 64760-21-0 64760-22-1 64760-23-2 **64760-24-3**
RL: BIOL (Biological study)
(in cigarette smoke condensate)

L33 ANSWER 44 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:503345 Document No. 87:103345 Synthesis of anthanthrene derivatives. Vorozhtsov, G. N.; Dokunikhin, N. S.; Fel'dblyum, N. B. (Nauchno-Issled. Inst. Org. Poluprod. Krasitelei, Moscow, USSR). Tezisy Vses. Simp. Org. Sint.: Benzoidnye Aromat. Soedin., 1st, 80-1. Akad. Nauk SSSR, Otd. Obshch. Tekh. Khim.: Moscow, USSR. (Russian) 1974. CODEN: 35COAS.
GI For diagram(s), see printed CA Issue.
AB Anthranthrenes I [X = CH2CH2 (II) [54481-13-9], CO2CO [54481-17-3], CONPhCO (III) [54481-19-5]] were prepared by cyclization of 6,6'-diacetyl-5,5'-biacenaphthene (IV) [21879-03-8], 5,5'-diacetyl-4,4'-bis(naphthalic anhydride) [54480-91-0], and 5,5'-diacetyl-N,N'-diphenyl-4,4'-binaphthalimide [54481-20-8], resp., in an acid medium; in the presence of reducing agents the yield was close to quant. III is a red-violet pigment. The bis(α-hydroxymethyl) derivative [54481-14-0] obtained by reduction of IV, upon cyclization, gave both the cis and trans isomers of the dihydro derivative of II and V.
IT **63118-20-7P 63118-21-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 63118-20-7 HCAPLUS
CN Dibenzo[def,mno]chrysene-3,4,9,10-tetracarboxylic acid, 6-methyl- (9CI) (CA INDEX NAME)

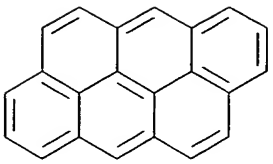


RN 63118-21-8 HCAPLUS
CN Dibenzo[def,mno]chrysene-3,4,9,10-tetracarboxylic acid, 6,12-dimethyl-, ion(4-) (9CI) (CA INDEX NAME)



CC 40-9 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
Section cross-reference(s): 26
IT 54481-13-9P 54481-17-3P 54481-19-5P 62799-25-1P 62799-27-3P **63118-20-7P 63118-21-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L33 ANSWER 45 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:499023 Document No. 87:99023 Correlation of polynuclear aromatic hydrocarbon formation between pyrolysis and smoking. Severson, R. F.; Schlotzhauer, W. S.; Arrendale, R. F.; Snook, M. E.; Higman, H. C. (Tob. Health Lab., ARS, Athens, GA, USA). Beitraege zur Tabakforschung, 9(1), 23-37 (English) 1977. CODEN: BETAAY. ISSN: 0005-819X.
AB Tobacco, its petroleum ether (PE) extract, and the residual extracted tobacco (marc) were pyrolyzed at 650-750°, 650-850°, and 700°, resp. Analyses of the polynuclear aromatic hydrocarbons (PAH) produced showed that the pyrolysis of the tobacco and the PE extract at 700° produced PAH profiles comparable to those found in cigarette smoke condensate. The data indicated that most of the alkyl PAH and the major PAH in cigarette smoke are derived from the PE extractables of tobacco. The constituents of the marc were the major precursors for phenols, oxygenated PAH, and low-mol.-weight acids; and those of the PE exts. were the major producers of high-mol.-weight acids.
IT **41699-10-9**
RL: BIOL (Biological study)
(in tobacco pyrolyzate, cigarette smoke composition in relation to)
RN 41699-10-9 HCAPLUS
CN Dibenzo[def,mno]chrysene, methyl- (9CI) (CA INDEX NAME)



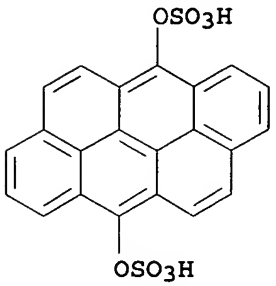
D1—Me

CC 11-7 (Plant Biochemistry)
IT 50-32-8, biological studies 53-70-3D, derivs. 56-55-3 83-32-9
85-01-8, biological studies 86-73-7 90-12-0 91-20-3,
biological studies 91-57-6 120-12-7, biological studies
129-00-0, biological studies 132-64-9 191-26-4 192-97-2
193-39-5 193-43-1 195-19-7 198-55-0 201-06-9 203-12-3D,
derivative 203-33-8 205-12-9 206-44-0 208-96-8 215-58-7
217-59-4 218-01-9 224-41-9D, derivs. 232-54-2 238-84-6
243-17-4 268-40-6 610-48-0 612-94-2 613-12-7 779-02-2
826-74-4 827-54-3 832-64-4 832-69-9 832-71-3 883-20-5
1430-97-3 1556-99-6 1730-37-6 2381-21-7 2523-37-7
2523-39-9 2531-84-2 3353-12-6 3442-78-2 7130-15-6
19345-99-4 20485-57-8 25167-89-9 25167-90-2 25732-74-5
25889-60-5 28652-77-9 28804-88-8 29062-98-4 29063-00-1
29348-63-8 30232-26-9 30582-03-7 33543-31-6 36541-21-6
41637-88-1 41637-90-5 41637-92-7 41699-04-1 41699-06-3
41699-09-6D, derivs. **41699-10-9** 43178-07-0 43178-22-9
56832-73-6D, derivative 58548-38-2 60684-29-9 60826-61-1
60826-62-2 60826-63-3 60826-64-4 60826-68-8 60826-74-6
60918-47-0 61261-04-9 64031-89-6 64031-90-9 64031-91-0
64082-72-0 64158-98-1 64158-99-2
RL: BIOL (Biological study)
(in tobacco pyrolyzate, cigarette smoke composition in relation to)

L33 ANSWER 46 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1977:163624 Document No. 86:163624 Stabilized photothermographic receptor film. Conder, Terrence M.; O'Leary, Kevin P. (Minnesota Mining and Manufacturing Co., USA). Ger. Offen. DE 2634893 19770217, 26 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1976-2634893 19760803.
AB In a modification of the process of U.S. 3,935,012 (Ger. Offen 2,433,831; CA 84: 67887x) a donor film contains a compound liberating a hydrogen halide during exposure to light, which in turn sets free a primary reductant from an acid-splittable precursor adduct (4-methoxy-1-naphthol-dihydropyran). The exposed film is contacted with a receptor sheet coated with a reducible metal soap (Ag behenate, Fe(III) stearate) and <25% of a phenolic reducing agent in a film-forming binder. Heating causes imagewise reduction of the soap to metal, catalyzed by the action of the primary reductant. To minimize the unwanted light-sensitivity of the receptor sheet it contains 0.007-0.5% (based on the metal salt) of a polycyclic dye with ≥1 solubilizing alkoxy or OH group. Thus, a receptor film coating was composed of Ag behenate dispersion, a cellulose propionate-poly(Et methacrylate) solution, 2,6-di-tert-butyl-p-cresol, and butylated Vat Violet 7.
IT **1324-23-8D**, butylated
RL: USES (Uses)

(photothermog. receptor sheet stabilized by)

RN 1324-23-8 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, diethoxy-, bis(hydrogen sulfate), disodium salt (8CI, 9CI) (CA INDEX NAME)

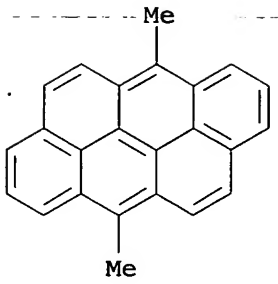


2 (D1—O—Et)

●2 Na

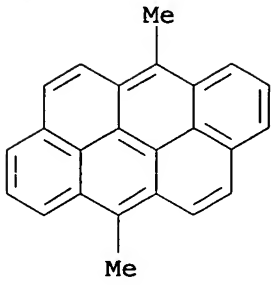
IC G03C001-72
CC 74-3 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT **1324-23-8D**, butylated 1324-54-5D, ethylated 4645-35-6
RL: USES (Uses)
(photothermog. receptor sheet stabilized by)

L33 ANSWER 47 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1976:145767 Document No. 84:145767 Dimethylnitrosamine-demethylase: molecular size-dependence of repression by polynuclear hydrocarbons. Nonhydrocarbon repressors. Arcos, Joseph C.; Valle, Ricardo T.; Bryant, Georgia M.; Buu Hoi, N. P.; Argus, Mary F. (Seamen's Mem. Res. Lab., U. S. Public Health Serv. Hosp., New Orleans, LA, USA). Journal of Toxicology and Environmental Health, 1(3), 395-408 (English) 1976. CODEN: JTEHD6. ISSN: 0098-4108.
AB Repression of dimethylnitrosamine demethylase [9075-31-4] in rat liver by i.p. injected polynuclear aromatic hydrocarbons required that the compds. satisfy specific requirements of mol. geometry with regard to size, shape, and coplanarity. Maximal repressor activity was associated with those planar compds. occupying a 2-dimensional area of 85-150 Å2. The hydrocarbons had to have an elongated rather than compact mol. shape, and coplanarity of the mol. was a critical requirement. A variety of compds. other than hydrocarbons also repressed the liver microsomal enzyme.
IT **41217-05-4**
RL: BIOL (Biological study)
(dimethylnitrosamine demethylase repression by, in liver microsomes)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 4-13 (Toxicology)
IT 50-32-8 53-70-3 56-49-5 56-55-3 57-97-6 81-31-2 83-32-9 85-01-8, biological studies 86-73-7 91-20-3, biological studies 92-24-0 120-12-7, biological studies 129-00-0, biological studies 188-73-8 189-55-9 189-64-0 190-26-1 190-70-5 190-72-7 191-07-1 191-24-2 191-26-4 191-30-0 191-68-4 191-87-7 192-47-2 192-51-8 192-58-5 192-65-4 192-97-2 193-39-5 198-55-0 205-99-2 207-83-0 208-96-8 213-46-7 214-17-5 215-58-7 215-96-3 217-54-9 217-59-4 218-01-9 224-41-9 227-09-8 238-84-6 239-98-5 275-51-4 540-61-4 604-59-1 781-43-1 1434-54-4 1981-38-0 2381-21-7 2541-69-7 3442-78-2 5385-75-1 6051-87-2 7646-79-9, biological studies 11097-69-1 **41217-05-4** 58706-01-7 58706-02-8
RL: BIOL (Biological study)
(dimethylnitrosamine demethylase repression by, in liver microsomes)

L33 ANSWER 48 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1976:73465 Document No. 84:73465 Simulated ab initio molecular orbital calculations of large polynuclear aromatic hydrocarbons. Duke, Brian J.; Eilers, Deidre R.; Eilers, James E.; Kang, Sungzong; Liberles, A.; O'Leary, Brian (Dep. Theor. Chem., Univ. Oxford, Oxford, UK). International Journal of Quantum Chemistry, Quantum Biology Symposium, 2, 155-70 (English) 1975. CODEN: IJQBDZ. ISSN: 0360-8832.
AB Mol. orbital electronic structure calcns. for twelve polynuclear aromatic hydrocarbons were performed by the SAMO method. Results indicate that the carcinogenicity of such aromatic hydrocarbons is related to a K-region π-bond order greater than 0.340. There is no correlation with σ-bond order or overall charge density, perhaps accounting for the success of earlier theor. treatments based on the π-electron model. Exceptions to a simple K-region treatment are discussed in terms of other models for carcinogenic activity.
IT **41217-05-4**
RL: PRP (Properties)
(MO calcns. for, carcinogenesis in relation to)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)

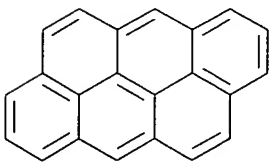


CC 22-8 (Physical Organic Chemistry)
IT 50-32-8 53-70-3 56-55-3 189-55-9 **41217-05-4**
RL: PRP (Properties)
(MO calcns. for, carcinogenesis in relation to)

L33 ANSWER 49 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1975:408591 Document No. 83:8591 Excited states of some organic charge transfer complexes studied by modulation excitation spectrophotometry. Slifkin, M. A.; Al-Chalabi, A. O. (Dep. Pure Appl. Phys., Univ. Salford, Salford, UK). Chemical Physics Letters, 30(2), 227-30 (English) 1975. CODEN: CHPLBC. ISSN: 0009-2614.
AB The excited states of some complexes between polycyclic aromatic hydrocarbons and chloranil dissolved in Me methacrylate polymer were studied with a modulation excitation spectrophotometer. New bands similar to, but slightly shifted in position as compared to, the T1-T3 transition of the aromatic hydrocarbon are observed Regressional anal. points to the new bands arising from transitions from a level in the chloranil to the T3 level of the hydrocarbon. An enhancement of the T1-T2 bands of the hydrocarbon occurs in the complex. Other bands are believed to be due to new levels of the complex which cannot be identified with local levels of the hydrocarbon or chloranil.
IT **56116-19-9**
RL: PRP (Properties)
(elec. parameters of)
RN 56116-19-9 HCAPLUS
CN 2,5-Cyclohexadiene-1,4-dione, 2,3,5,6-tetrachloro-, compd. with dibenzo[def,mno]chrysene (2:1) (9CI) (CA INDEX NAME)

CM 1

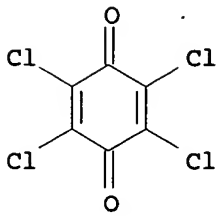
CRN 191-26-4
CMF C22 H12



CM 2

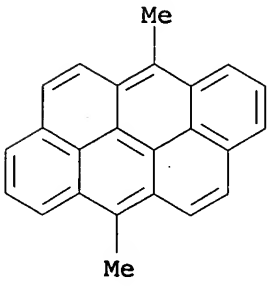
CRN 118-75-2

CMF C6 Cl4 O2



CC 22-2 (Physical Organic Chemistry)
IT 56-55-3 191-07-1 191-24-2 191-26-4 213-46-7 214-17-5
218-01-9 517-51-1 56058-81-2 56058-82-3 56058-83-4
56058-84-5 56058-85-6 56058-86-7 56058-87-8 **56116-19-9**
RL: PRP (Properties)
(elec. parameters of)

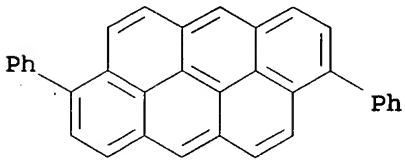
L33 ANSWER 50 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1975:169771 Document No. 82:169771 Reactivity of polycyclic aromatic hydrocarbons in light-initiated degradation. Paalme, L.; Tuulmets, A.; Kirso, U.; Gubergrits, M. (Inst. Chem., Tallinn, USSR). Reaktsionnaya Sposobnost Organicheskikh Soedinenii, 11(2), 315-24 (English) 1974. CODEN: RSOTAY. ISSN: 0375-9520.
AB The pseudo-0 order rate consts. of the light-initiated decomposition of twenty-seven polycyclic aromatic hydrocarbons (including benzopyrenes, phenanthrene, coronene, fluorene, and methylcholanthrene) in C6H6 were determined under O or argon. The rate consts. were linearly related with several MO indexes and the Streitwieser $\sigma\gamma$ consts. The reaction rate was weakly sensitive to the changes in electron d. at the reaction center. The more reactive the hydrocarbon the more carcinogenic it was.
IT **41217-05-4**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(photodecompn. of, kinetics of)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 22-7 (Physical Organic Chemistry)
Section cross-reference(s): 6
IT 50-32-8 53-70-3 56-49-5 56-55-3 57-97-6 85-01-8, reactions
86-73-7 92-24-0 129-00-0, reactions 191-07-1 191-24-2
191-30-0 192-97-2 198-55-0 215-58-7 217-59-4 218-01-9
224-41-9 2381-39-7 2422-79-9 2498-75-1 2541-69-7

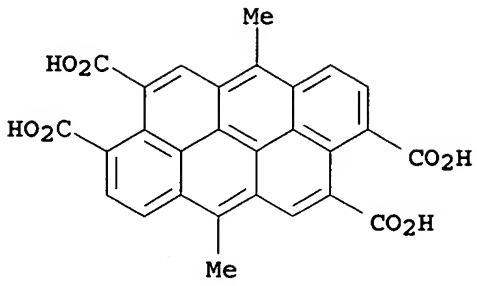
40568-90-9 40568-91-0 40568-92-1 40568-93-2 **41217-05-4**
RL: PRP (Properties); RCT (Reactant); RACT (Reactant or reagent)
(photodecompn. of, kinetics of)

L33 ANSWER 51 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1975:139830 Document No. 82:139830 New benzenogenic diene syntheses. Clar, E.; Lovat, M. M.; Simpson, W. (Dep. Chem., Univ. Glasgow, Glasgow, UK). Tetrahedron, 30(18), 3293-8 (English) 1974. CODEN: TETRAB. ISSN: 0040-4020.
GI For diagram(s), see printed CA Issue.
AB 1,5-Dibenzylnaphthalene with excess maleic anhydride in the presence of PhNO2 and iodine gave 3,8-diphenylpyrene-4,5:9,10-tetracarboxylic dianhydride which was decarboxylated (basic Cu carbonate in quinoline) to 3,8-diphenylpyrene (I). Similarly, 3,10-diphenylpyrene, 3,9-diphenylanthranthrene, 4,9-diphenyl-1,12-benzoperylene (II), and 1,6-diphenylcoronene were prepared from 1,4-dibenzylnaphthalene, 3,8-dibenzylpyrene, 3,10-dibenzylpyrene, and II, resp.
IT **54811-25-5P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 54811-25-5 HCAPLUS
CN Dibenzo[def,mno]chrysene, 3,9-diphenyl- (9CI) (CA INDEX NAME)



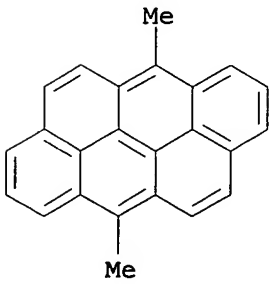
CC 26-6 (Condensed Aromatic Compounds)
IT 54811-22-2P 54811-23-3P **54811-25-5P** 54811-28-8P
55009-75-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

L33 ANSWER 52 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1975:113191 Document No. 82:113191 Anthanthrenes. Dokunikhin, N. S.; Vorozhtsov, G. N.; Kichina, F. I.; Fel'dblyum, N. B. Ger. Offen. DE 2318285 19741031, 20 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1973-2318285 19730411.
GI For diagram(s), see printed CA Issue.
AB Six anthanthrenes I [R, R1 = CO2H; or (RR1) = CH2CH2, CO2CO, CONPhCO, or R3; R2 = Me or Et], useful as intermediates for dyes and as dyes, were prepared from 1,1'-binaphthyl derivs. Thus, the binaphthyl derivative (II) [54480-91-0] was heated in H3PO4 containing POCl3 at 145° to give 86% 6,12-dimethyl-3,4:9,10-anthanthrenetetracarboxylic dianhydride [54481-17-3]. Similarly prepared were 4 addnl. I. Heating II and o-(H2N)2C6H4 [95-54-5] in 75% H2SO4 at 70° gave 85% dark-blue dye I [(RR1) = R3, R2 = Me] [54481-21-9].
IT **54481-18-4P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 54481-18-4 HCAPLUS
CN Dibenzo[def,mno]chrysene-3,4,9,10-tetracarboxylic acid, 6,12-dimethyl- (9CI) (CA INDEX NAME)



IC C09B; C07C; C07D
CC 40-10 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
Section cross-reference(s): 26
IT 54481-13-9P 54481-15-1P 54481-17-3P **54481-18-4P**
54481-19-5P 54481-21-9P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

L33 ANSWER 53 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1975:66664 Document No. 82:66664 Crystal and molecular structure of 6,12-dimethyldibenzo[def,mno]chrysene (6,12-dimethylanthanthrene). Iball, John; Scrimgeour, Sheelagh N. (Chem. Dep., Univ. Dundee, Dundee, UK). Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (12), 1445-8 (English) 1974. CODEN: JCPKBH. ISSN: 0300-9580.
GI For diagram(s), see printed CA Issue.
AB Crystals of the title compound (I) were monoclinic, space group P21/c, with a 22.17, b 5.229, c 13.458 A, β 105.21°, d. (observed) 1.334, and d. (calculated) 1.341 for Z = 4; R was 0.087 from 1725 observed reflections. The 2 independent centrosym. mols in the unit cell were planar and did not differ significantly.
IT **41217-05-4**
RL: PRP (Properties)
(crystal structure of)
RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



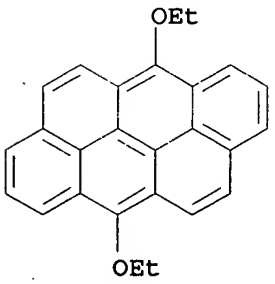
CC 75-5 (Crystallization and Crystal Structure)
IT **41217-05-4**
RL: PRP (Properties)
(crystal structure of)

L33 ANSWER 54 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1974:471107 Document No. 81:71107 Photosensitive material containing a diaryliodium compound, a sensitizer and a color former. Smith, George H. (Minnesota Mining and Manufacturing Co.). U.S. US 3808006 19740430, 5 pp. Division of U. S. 3,729,313 (CA 79;131408t). (English). CODEN: USXXAM. APPLICATION: US 1973-346064 19730329.

AB Free-radical printout photog. materials containing a diaryliodonium compound, such as diphenyliodonium bis(trifluorosulfonyl)methide (I), an aminotriarylmethane photosensitizer, and a color forming reactant capable of color formation in the presence of free radicals are described. Thus, 5 parts of a solution containing pentaerythritol tetraacrylate 100, a 20% dispersion of finely divided Ni stearate in MeCOEt 167, I 3.34, and Thioflavin T 0.2 parts were coated on a polyester support, dried, laminated to a 2 mil polyester film, exposed through a stencil to a W-light (15,000 ft-candles) for 6 sec, peeled apart and the top film contacted with a receptor paper coated with 20 parts of a 5% solution of Et cellulose in Me2CO containing 0.1 parts of dibenzyldithiooxamide. After transfer, the paper was heated at 100° for 10 sec to give a dark purple pos. copy of the original.

IT **53332-39-1**
RL: USES (Uses)
(photosensitizer, photog. silver-free print-out emulsions containing diphenyliodonium compds., trimethylolpropane trimethacrylate, and)

RN 53332-39-1 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-diethoxy- (9CI) (CA INDEX NAME)



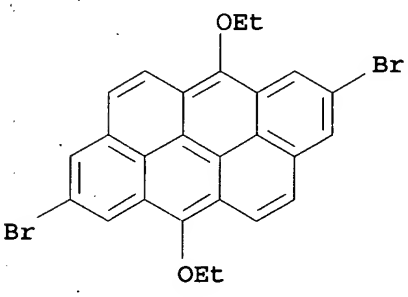
IC G03C
NCL 096088000
CC 74-8 (Radiation Chemistry, Photochemistry, and Photographic Processes)
IT 81-93-6 87-01-4 531-53-3 905-96-4 1030-27-9 1612-64-2 1628-58-6 2465-29-4 5522-66-7 38097-28-8 50721-67-0 50721-68-1 50721-69-2 50721-70-5 50721-71-6 50834-70-3 50866-65-4 **53332-39-1**
RL: USES (Uses)
(photosensitizer, photog. silver-free print-out emulsions containing diphenyliodonium compds., trimethylolpropane trimethacrylate, and)

L33 ANSWER 55 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1973:406803 Document No. 79:6803 Polycyclic aromatic dyes. Burleigh, Malcolm B. (Minnesota Mining and Manufacturing Co.). Ger. Offen. DE 2245233 19730329, 26 pp. (German). CODEN: GWXXBX. APPLICATION: DE 1972-2245233 19720912.

AB Stable, soluble polycyclic aromatic sensitizing dyes containing at least two

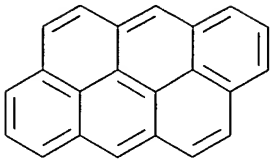
linear three catacondensed benzene rings containing ethoxy groups in the meso position and halogen substituted were prepared and were used in copying processes. These dyes contain 6, 8, and 9 rings. Thus, C.I. Vat Blue 18 [1324-54-5] was heated with aqueous -NaOH and Na2S2O4 in Me2CHOH and then treated with Et2SO4 to give polycyclic dye (I) [40537-72-2]. I in the presence of light and O destroys 1,3-diphenylisobenzofuran acceptor. The other I were similarly prepared

IT **42803-67-8P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)
RN 42803-67-8 HCAPLUS
CN Dibenzo[def,mno]chrysene, 2,8-dibromo-6,12-diethoxy- (9CI) (CA INDEX NAME)



IC C09B
CC 40-13 (Dyes, Fluorescent Whitening Agents, and Photosensitizers)
IT 40537-72-2P 42803-65-6P 42803-66-7P **42803-67-8P**
42803-68-9P
RL: IMF (Industrial manufacture); PREP (Preparation)
(preparation of)

L33 ANSWER 56 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1973:163517 Document No. 78:163517 Application of a gas chromatograph-mass spectrometer-data processor combination to the analysis of the polycyclic aromatic hydrocarbon content of airborne pollutants. Lao, R. C.; Thomas, R. S.; Oja, H.; Dubois, L. (Air Polut. Control Dir., Dep. Environ., Ottawa, ON, Can.). Analytical Chemistry, 45(6), 908-15 (English) 1973. CODEN: ANCHAM. ISSN: 0003-2700.
AB A gas chromatog.-mass spectrometer (GC-MS) data system was used to measure polynuclear aromatic hydrocarbons (PAH) in air samples. Airborne particulate samples were collected on glass fiber filters using a high volume sampler. The filters were Soxhlet-extracted using cyclohexane, and extractable matter was Rosen-separated The PAH fraction was concentrated and injected into the GC-MS system. For each GC peak, mass spectra were obtained and compared to PAH reference stds. with the separation and identification of >70 major PAH having from 2 to 7 rings in an air sample. Samples of <100 μg produced good data for the individual components emerging from the column in amts. in the ng region.
IT **41699-10-9**
RL: ANT (Analyte); ANST (Analytical study)
(determination of)
RN 41699-10-9 HCAPLUS
CN Dibenzo[def,mno]chrysene, methyl- (9CI) (CA INDEX NAME)



D1—Me

CC 59-2 (Air Pollution and Industrial Hygiene)
Section cross-reference(s): 51, 52

IT 50-32-8 56-49-5 56-55-3 57-97-6 57-97-6 85-01-8, analysis
86-73-7 92-52-4, analysis 120-12-7, analysis 129-00-0,
analysis 135-48-8 191-07-1 191-24-2 191-26-4 191-30-0
192-65-4 192-97-2 193-39-5 193-43-1 195-19-7 198-55-0
203-12-3 205-12-9 205-82-3 205-99-2 206-44-0 207-08-9
213-46-7 214-17-5 215-58-7 217-59-4 218-01-9 232-54-2
238-84-6 243-17-4 260-36-6 260-94-6 316-49-4 612-78-2
613-12-7 613-31-0 776-35-2 832-71-3 1079-71-6 1430-97-3
1730-37-6 2523-37-7 2523-48-0 2531-84-2 25167-89-9
25167-90-2 27577-90-8 28652-72-4 28779-32-0 29062-98-4
29063-00-1 29966-04-9 30283-95-5 30997-38-7 31423-95-7
33543-31-6 39379-95-8 39379-96-9 39380-03-5 39380-04-6
39380-05-7 39380-06-8 39380-13-7 41593-21-9 41593-22-0
41593-23-1 41593-24-2 41593-25-3 41593-26-4 41593-27-5
41593-28-6 41593-29-7 41593-30-0 41593-31-1 41637-86-9
41637-87-0 41637-88-1 41637-89-2 41637-90-5 41637-91-6
41637-92-7 41637-93-8 41637-94-9 41667-60-1 41699-04-1
41699-05-2 41699-06-3 41699-07-4 41699-08-5 41699-09-6
41699-10-9 41724-32-7
RL: ANT (Analyte); ANST (Analytical study)
(determination of)

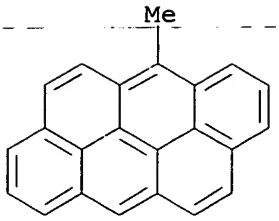
L33 ANSWER 57 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1973:42354 Document No. 78:42354 Nature of para bond and of para coupling [in polyaceneS]. Clar, E.; Mackay, C. C. (Dep. Chem., Univ. Glasg., Glasgow, UK). Tetrahedron, 28(19), 5049-54 (English) 1972. CODEN: TETRAB. ISSN: 0040-4020.

AB The PMR coupling in anthracene and tetracene derivs. was studied by spin-spin decoupling methods; the para coupling in the middle ring of these compds. was too small to be measured. There was no peri or epi coupling between meso positions, however there was appreciable coupling between meso and terminal peri positions. A very weak para π-bond was assumed; this was strengthened in meso-Me derivs. and became comparable with the π-bond between meso C atoms in phenanthrene. The meso-Me signals were split into doublets by the para protons; e.g. the coupling constant was 0.8 Hz for 1-chloro-10-methyl-anthracene.

IT **31927-64-7**
RL: PRP (Properties)
(NMR of)

RN 31927-64-7 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

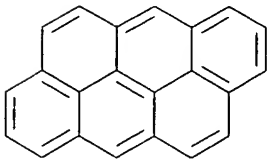


CC 22-2 (Physical Organic Chemistry)
IT 90-12-0 571-61-9 610-48-0 883-20-5 954-07-4 2381-31-9
4076-43-1 4626-38-4 4985-70-0 14214-56-3 15815-48-2
21297-24-5 **31927-64-7** 40577-76-2 40577-77-3
40577-78-4
RL: PRP (Properties)
(NMR of)

L33 ANSWER 58 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1972:105910 Document No. 76:105910 Vibrational studies of aromatic hydrocarbon-trinitrobenzene charge-transfer complexes. Larkindale, J. P.; Simkin, D. J. (Chem. Dep., McGill Univ., Montreal, QC, Can.). Spectrochimica Acta, Part A: Molecular and Biomolecular Spectroscopy, 28(3), 485-91 (English) 1972. CODEN: SAMCAS. ISSN: 1386-1425.
AB A vibrational study of aromatic hydrocarbon-trinitrobenzene charge-transfer complexes was carried out to investigate changes due to complexation. Small frequency shifts were observed in solid phase spectra, but not in solution studies. An explanation of the exptl. data is offered.
IT **34892-84-7**
RL: PRP (Properties)
(vibrational spectrum of)
RN 34892-84-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, compd. with 1,3,5-trinitrobenzene (1:1) (9CI) (CA INDEX NAME)

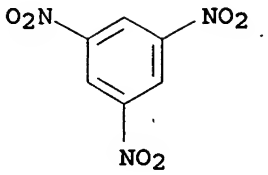
CM 1

CRN 191-26-4
CMF C22 H12



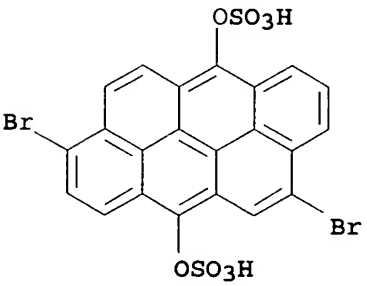
CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



CC 73 (Spectra by Absorption, Emission, Reflection, or Magnetic Resonance, and Other Optical Properties)
IT 980-80-3 1700-13-6 1787-27-5 15251-37-3 34892-82-5 **34892-84-7** 34892-85-8 34892-86-9
RL: PRP (Properties)
(vibrational spectrum of)

L33 ANSWER 59 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1967:56576 Document No. 66:56576 Alkali metal salts of the acid sulfate esters of leuco vat dyes. Khoroshun, M. M.; Antonenko, G. B.; Perevoznik, A. I. U.S.S.R. SU 185429 19660813 From: Izobret., Prom. Obraztsy, Tovarnye Znaki 1966, 43(17), 51. (Russian). CODEN: URXXAF. APPLICATION: SU 19630330.
AB To increase the solubility and stability of the dyes the salts are prepared by treating an aqueous paste of the title salts with trioloxide followed by distillation of water in vacuum.
IT **15887-47-5P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(stable preparation of)
RN 15887-47-5 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,9-dibromo-, bis(hydrogen sulfate), disodium salt (8CI) (CA INDEX NAME)



●2 Na

IC C09B
CC 40 (Dyes, Fluorescent Brightening Agents, and Photosensitizers)
IT 4425-36-9P 15114-99-5P **15887-47-5P**
RL: IMF (Industrial manufacture); PREP (Preparation)
(stable preparation of)

L33 ANSWER 60 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1964:410876 Document No. 61:10876 Original Reference No. 61:1731f-h The charge-transfer interaction in solid molecular complexes. Kuroda, H.; Yoshihara, K.; Kinoshita, M.; Akamatu, H. (Univ. Tokyo). Proc. Intern. Symp. Mol. Struct. Spectry., Tokyo (D101), 4pp

(Unavailable) 1962.

AB Charge-transfer (CT) complexes are classified into (1) those with weak interaction e.g., of polycyclic aromatic hydrocarbons and trinitrobenzene or tetracyanoethylene, (2) those with moderate interaction e.g., of PhNMe2 and chloranil or bromanil, (3) those with a strong interaction e.g., of I with polycyclic aroms., and (4) ionic complexes e.g., of SbCl5 with polycyclic aroms. In 1, the CT band in the solid state is red-shifted compared to the solution band of the 1:1 complex. They do not show ESR (ESR) absorption at room temperature and are poor elec. conductors, but show photoconduction. Linear plots are obtained between the energy gap (E) and the energy of CT excitation (hvCT). In 2, the CT band of the solid complex is considerably blue-shifted compared to the solution data. It possesses appreciable conductivity but weak ESR absorption. Type 3 complexes usually show strong ESR absorption, remarkable conductivity, and very broad absorption spectra different from the solution spectra of the complexes or of the pos. donor ions. In 4, due to strong CT interaction, the solid complex contains pos. donor ions and neg. acceptor ions. It shows strong ESR absorption from which the % ionization may be calculated The spectrum of the solid complex resembles that of the pos. donor ion in solution For 1, $\varepsilon \approx h\nu_{CT}$; for 2, $\varepsilon \ll h\nu_{CT}$.

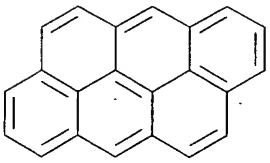
IT **34892-84-7**, Dibenzo[def,mno]chrysene, compound with 1,3,5-trinitrobenzene (1:1)
(electron transfer in)

RN 34892-84-7 HCAPLUS

CN Dibenzo[def,mno]chrysene, compd. with 1,3,5-trinitrobenzene (1:1) (9CI) (CA INDEX NAME)

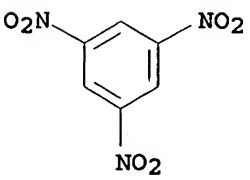
CM 1

CRN 191-26-4
CMF C22 H12



CM 2

CRN 99-35-4
CMF C6 H3 N3 O6



CC 32 (Physical Organic Chemistry)

IT 1223-66-1, Naphthalene, compound with ethenetetracarbonitrile (1:1)

1223-66-1, Ethenetetracarbonitrile, compound with naphthalene (1:1)
1700-13-6, Anthracene, compound with 1,3,5-trinitrobenzene (1:1)
2399-97-5, Pyrene, compound with ethenetetracarbonitrile (1:1)
2876-91-7, Perylene, compound with ethenetetracarbonitrile (1:1)
2876-95-1, Pyrene, compound with I2 (1:2) 2877-00-1, Perylene, compound with I2 (2:3) 3445-48-5, p-Benzoquinone, tetrachloro-, compound with N,N-dimethylaniline 6164-86-9, Pyrene, compound with 1,3,5-trinitrobenzene (1:1) 6418-68-4, Perylene, compound with SbCl5 15251-37-3, Perylene, compound with 1,3,5-trinitrobenzene (1:1) 16636-09-2, Aniline, N,N-dimethyl-, compound with 1,3,5-trinitrobenzene 18273-63-7, Antimony chloride, SbCl5, compound with phenanthrene 18273-67-1, Antimony chloride, SbCl5, compound with anthracene 18274-05-0, Antimony chloride, SbCl5, compound with phenothiazine 18274-09-4, Antimony chloride, SbCl5, compound with pyrene 20265-16-1, Chrysene, compound with 1,3,5-trinitrobenzene (1:1) 22011-63-8, p-Benzoquinone, tetrabromo-, compound with N,N-dimethylaniline 25158-57-0, Phenanthrene, compound with ethenetetracarbonitrile 25724-19-0, Phenothiazine, compound with I2 (1:1) 29271-85-0, Phenanthrene, compound with 1,3,5-trinitrobenzene **34892-84-7**, Dibenzo[def,mno]chrysene, compound with 1,3,5-trinitrobenzene (1:1)
(electron transfer in)

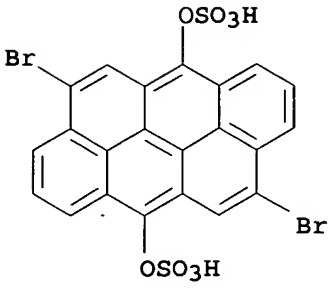
L33 ANSWER 61 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1964:75868 Document No. 60:75868 Original Reference No. 60:13376c-e
Photoreaction of the H2SO4 esters of leuco vat dyes. Dobozy, Otto; Marosi, Jozsef (Kozponti Kolorisztikai Kutato Lab., Budapest, Hung.). Kolorisztikai Ertesito, 5(5), 222-37 (Unavailable) 1963. CODEN: KOERA9. ISSN: 0023-2939.

AB The H2SO4 esters of the dyes are converted to their oxo forms on exposure to light; this reaction is useful in making possible the formation of new colored patterns on textiles, but it also makes useless part or all of expensive dyes by unwanted exposure. The esters (22) were investigated under controlled conditions of exposure to light. Development of maximum depth of color depended upon the length of exposure with some dyes, but was independent with others. A correlation between chemical structure and photosensitivity was established and the following order of decreasing sensitivity was found: thioindigo derivs., indigo derivs., substituted anthraquinones, polynuclear aromatic ketones. The anthraquinone-azine derivs. are not photosensitive. It is assumed that during the process of photooxidn. the total structure participates rather than only the ester groups. The role of the catalyst was also studied by examining 18 inorg. and organic substances in the photooxidn. of these dyes. The greatest catalytic effects were exhibited by substances which are well-known light inhibitors. Lesser effects were exhibited by reduction-oxidation and acid-base inhibitors. Certain filters and long-wavelength light were effective in eliminating undesirable pigment-forming reactions.

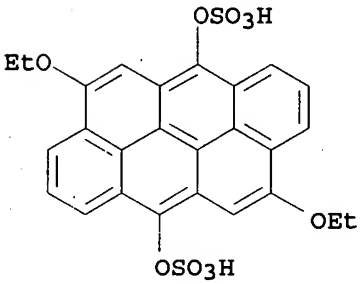
IT **4378-58-9**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) **4378-59-0**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-diethoxy-, bis(hydrogen sulfate)
(photochem. oxidation of)

RN 4378-58-9 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) (8CI, 9CI) (CA INDEX NAME)



RN 4378-59-0 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-diethoxy-, bis(hydrogen sulfate) (9CI) (CA INDEX NAME)



CC 47 (Textiles)
IT 2678-71-9, Dinaphtho[1,2,3-cd:3',2',1'-lm]perylene-5,10-diol, 16,17-dimethoxy-, bis(hydrogen sulfate) **4378-58-9**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) **4378-59-0**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-diethoxy-, bis(hydrogen sulfate) 4388-08-3, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6-chloro-6'-methoxy-4-methyl-, bis(hydrogen sulfate) 4388-10-7, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6,6'-dichloro-4,4'-dimethyl-, bis(hydrogen sulfate) 4388-11-8, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6,6'-diethoxy-, bis(hydrogen sulfate) 4388-12-9, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 5,6',7-trichloro-4,4'-dimethyl-, bis(hydrogen sulfate) 4568-45-0, Anthra[2,3-d]oxazole-5,10-diol, 2-(1-amino-9,10-dihydroxy-2-anthryl)-, tetrakis(hydrogen sulfate) (ester) 5632-11-1, Hydroquinone, 2,5-bis(p-chloroanilino)-, bis(hydrogen sulfate (ester) 6371-40-0, [2,2'-Biindole]-3,3'-diol, 5,6',7-trichloro-, bis(hydrogen sulfate) (ester) 6406-16-2, Naphtho[2,3-b]thiophene-3-ol, 9-chloro-2-(3-hydroxybenzo[b]thien-2-yl)-, bis(hydrogen sulfate) 6527-57-7, 4-Biphenylcarboxamide, N-(9,10-dihydroxy-1-anthryl)-, bis(hydrogen sulfate) 6897-40-1, 5,9,14,18-Anthrazinetetrol, 7,16-dichloro-6,15-dihydro-, tetrakis(hydrogen sulfate) (ester) 25666-23-3, 11H-Benzo[a]carbazol-4-ol, 3-(3-hydroxyindol-2-yl)-10-methyl-, bis(hydrogen sulfate) (ester) 25740-98-1, [2,2'-Biindole]-3,3'-diol, 5,5',7,7'-tetrabromo-, bis(hydrogen sulfate) (ester) 93941-72-1, Dibenzo[b,def]chrysene-7,14-diol, dibromo-, bis(hydrogen sulfate) 121991-36-4, Benzamide, N,N'-(9,10-dihydroxy-1,5-anthrylene)bis-, bis(hydrogen sulfate)
(photochem. oxidation of)

L33 ANSWER 62 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1964:64994 Document No. 60:64994 Original Reference No. 60:11441f-g
X-ray powder diffraction patterns of solid hydrocarbons, derivatives of hydrocarbons, phenols, and organic bases. Hofer, L. J. E.; Peebles, W. C.; Bean, E. H. (U.S. Bur. of Mines, Washington, DC). Bulletin - United States, Bureau of Mines, No. 613, 59 pp. (Unavailable) 1963. CODEN: XBMBAJ. ISSN: 0082-9129.

AB Included are compds. of interest in research involving fuels, coal tar dyes, plastics, pharmaceutical, agricultural chems., carcinogens, air pollutants, and other public health problems. X-ray powder diffraction patterns (178) are presented of aromatic hydrocarbons, 2,4,7-trinitro-9-fluorenone derivs. of aromatic hydrocarbons, phenols, and organic bases for pos. identification of solid organic compds.

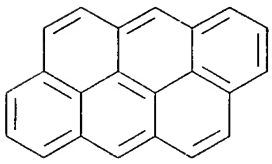
IT **96674-12-3**, Dibenzo[def,mno]chrysene, compound with 2,4,7-trinitrofluoren-9-one (1:1)
(x-ray diffraction pattern for)

RN 96674-12-3 HCAPLUS

CN Dibenzo[def,mno]chrysene, compd. with 2,4,7-trinitrofluoren-9-one (1:1) (7CI) (CA INDEX NAME)

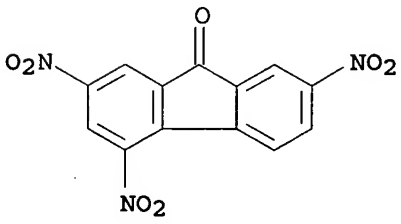
CM 1

CRN 191-26-4
CMF C22 H12



CM 2

CRN 129-79-3
CMF C13 H5 N3 O7



CC 8 (Crystallization and Crystal Structure)

IT 56-49-5, Cholanthrene, 3-methyl- 56-55-3, Benz[a]anthracene 60-09-3, C.I. Solvent Yellow 1 61-54-1, Indole, 3-(2-aminoethyl)- 66-71-7, 1,10-Phenanthroline 67-51-6, Pyrazole, 3,5-dimethyl- 80-46-6, Phenol, p-tert-pentyl- 83-32-9, Acenaphthene 83-34-1, Indole, 3-methyl-(skatole) 84-67-3, Benzidine, 2,2'-dimethyl- 85-01-8, Phenanthrene 85-02-9, Benzo[f]quinoline 85-06-3, Benzo[f] quinoline, 3-methyl- 86-73-7, Fluorene 86-74-8, Carbazole 87-66-1, Pyrogallol 89-83-8, Thymol 90-12-0, Naphthalene,

1-methyl- 90-15-3, 1-Naphthol 90-43-7, Phenol, o-phenyl- 90-45-9, Acridine, 9-amino- 91-20-3, Naphthalene 91-57-6, Naphthalene, 2-methyl- 91-59-8, 2-Naphthylamine 91-77-0, Melamine, N2,N2-diallyl- 92-67-1, 4-Biphenylamine 92-69-3, Phenol, p-phenyl- 92-82-0, Phenazine 92-87-5, Benzidine 92-94-4, p-Terphenyl 95-20-5, Indole, 2-methyl- 95-54-5, o-Phenylenediamine 95-55-6, Phenol, o-amino- 95-65-8, 3,4-Xylenol 95-87-4, 2,5-Xylenol 96-76-4, Phenol, 2,4-di-tert-butyl- 98-54-4, Phenol, p-tert-butyl- 100-97-0, Hexamethylenetetramine 101-01-9, Guanidine, 1,2,3-triphenyl- 101-54-2, p-Phenylenediamine, N-phenyl- 102-06-7, Guanidine, 1,3-diphenyl- 103-29-7, Bibenzyl 103-33-3, Azobenzene (benzeneazobenzene) 106-49-0, p-Toluidine 106-50-3, p-Phenylenediamine 108-45-2, m-Phenylenediamine 108-46-3, Resorcinol 108-68-9, 3,5-Xylenol 108-73-6, Phloroglucinol 108-78-1, Melamine 108-80-5, s-Triazine-2,4,6(1H,3H,5H)-trione 108-95-2, Phenol 119-42-6, Phenol, o-cyclohexyl- 119-64-2, Naphthalene, 1,2,3,4-tetrahydro- 119-91-5, 2,2'-Biquinoline 120-72-9, Indole 120-80-9, Pyrocatechol 122-66-7, Hydrazobenzene 123-30-8, Phenol, p-amino- 123-31-9, Hydroquinone 128-37-0, p-Cresol, 2,6-tert-butyl- 129-00-0, Pyrene 129-73-7, Aniline, 4,4'-benzylidenebis[N,N-dimethyl- 129-79-3, Fluoren-9-one, 2,4,7-trinitro- 134-32-7, 1-Naphthylamine 135-19-3, 2-Naphthol 135-88-6, 2-Naphthylamine, N-phenyl- 136-77-6, Resorcinol, 4-hexyl- 153-78-6, Fluoren-2-amine 191-24-2, Benzo[ghi]perylene 191-26-4, Dibenzo[def,mno]chrysene 198-55-0, Perylene 203-64-5, 4H-Cyclopenta[def]phenanthrene 205-12-9, 7H-Benzo[c]fluorene 218-01-9, Chrysene 238-84-6, 11H-Benzo[a]fluorene 260-94-6, Acridine 271-63-6, 1H-Pyrrolo[2,3-b]pyridine 288-32-4, Imidazole 366-18-7, 2,2'-Bipyridine 479-23-2, Cholanthrene 484-17-3, 9-Phenanthrol 497-39-2, m-Cresol, 4,6-di-tert-butyl- 501-24-6, Phenol, m-pentadecyl- 504-15-4, Resorcinol, 5-methyl- 504-24-5, Pyridine, 4-amino- 504-29-0, Pyridine, 2-amino- 519-73-3, Methane, triphenyl- 529-35-1, 1-Naphthol, 5,6,7,8-tetrahydro- 538-51-2, Aniline, N-benzylidene- 576-26-1, 2,6-Xylenol 588-53-4, Phenol, p-(benzylideneamino)- 588-59-0, Stilbene 591-27-5, Phenol, m-amino- 599-64-4, Phenol, p-(α,α-dimethylbenzyl)- 603-34-9, Triphenylamine 604-53-5, 1,1'-Binaphthyl 605-55-0, 2-Phenanthrol 612-78-2, 2,2'-Binaphthyl 612-95-3, Quinoline, 6-phenyl- 613-31-0, Anthracene, 9,10-dihydro- 613-33-2, p,p'-Bitolyl 616-55-7, o-Cresol, 4,6-di-tert-butyl- 618-45-1, Phenol, m-isopropyl- 621-09-0, Acetamidine, N,N'-diphenyl- 622-15-1, Formamidine, N,N'-diphenyl- 695-34-1, 4-Picoline, 2-amino- 697-82-5, Phenol, 2,3,5-trimethyl- 698-71-5, m-Cresol, 5-ethyl- 732-26-3, Phenol, 2,4,6-tri-tert-butyl- 827-54-3, Naphthalene, 2-vinyl- 873-74-5, Benzonitrile, p-amino- 877-43-0, Quinoline, 2,6-dimethyl- 883-20-5, Phenanthrene, 9-methyl- 886-65-7, 1,3-Butadiene, 1,4-diphenyl- 933-67-5, Indole, 7-methyl- 948-65-2, Indole, 2-phenyl- 1004-38-2, Pyrimidine, 2,4,6-triamino- 1079-71-6, Anthracene, 1,2,3,4,5,6,7,8-octahydro- 1125-78-6, 2-Naphthol, 5,6,7,8-tetrahydro- 1131-60-8, Phenol, p-cyclohexyl- 1135-32-6, Pyridine, 4,4'-vinylenedi- 1140-29-0, Ethylenediamine, N,N-diphenyl- 1195-46-6, Phenol, p-(ethylthio)- 1470-94-6, 5-Indanol 1556-99-6, Fluorene, 4-methyl- 1603-41-4, 3-Picoline, 6-amino- 1641-41-4, 4-Indanol 1705-85-7, Chrysene, 6-methyl- 1806-26-4, Phenol, p-octyl- 1824-81-3, 2-Picoline, 6-amino- 1885-29-6, Anthranilonitrile 1988-89-2, Phenol, p-(α-methylbenzyl)- 2141-42-6, Anthracene, 1,2,3,4-tetrahydro- 2219-84-3, o-Cresol, 4-(1,1,3,3-

tetramethylbutyl)- 2379-55-7, Quinoxaline, 2,3-dimethyl-
2433-56-9, 1-Phenanthrol 2443-58-5, Fluoren-2-ol 2523-37-7,
Fluorene, 9-methyl- 2717-42-2, Naphthalene, 1,2,4-trimethyl-
2732-58-3, Chrysene, 6-ethyl- 3228-01-1, o-Cymen-3-ol 3228-02-2,
o-Cymen-5-ol 3228-03-3, m-Cymen-5-ol 3324-27-4, Fluoren-9-one,
2,4,7-trinitro-, compound with perylene(1:1) 3324-30-9,
Fluoren-9-one, 2,4,7-trinitro-, compound with phenanthrene (1:1)
3353-12-6, Pyrene, 4-methyl- 3357-37-7, Guanidine,
(benzylideneamino)- 3558-24-5, Indole, 1-methyl-2-phenyl-
3697-24-3, Chrysene, 5-methyl- 3697-27-6, Chrysene, 5,6-dimethyl-
3710-23-4, Naphthalene, 2-isopropenyl- 3918-78-3, Fluoren-9-one,
2,4,7-trinitro-, compound with pyrene (1:1) 4044-57-9, Naphthalene,
1-(phenylethynyl)- 4130-42-1, Phenol, 2,6-di-tert-butyl-4-ethyl-
4325-74-0, 1,2'-Binaphthyl 4325-77-3, Phenanthrene, 2-phenyl-
4482-03-5, Bimesityl 4511-99-3, as-Triazine, 3-amino-5,6-diphenyl-
4518-00-7, Phenol, o-isobornyl- 5315-79-7, 1-Pyrenol 5405-13-0,
o-Toluidine, N-benzyl- 5412-43-1, 4-Biphenylamine, N,N-diethyl-
5427-08-7, Phenol, 2,6-di-tert-butyl-4-cyclohexyl- 6344-61-2,
Fluoren-1-ol 6628-98-4, Pyrene, 4,5-dihydro- 6876-33-1,
Benzonitrile, 2,2',2''-s-triazine-2,4,6-triyltri- 7499-40-3,
Picene, 5-methyl- 15300-67-1, 2,2'-Binaphthyl, compound with
2,4,7-trinitrofluoren-9-one 15658-11-4, Methanol,
(p-hydroxyphenyl)diphenyl- 20265-02-5, Fluoren-9-one,
2,4,7-trinitro-, compound with fluorene(1:1) 20265-03-6, Chrysene,
compound with 2,4,7-trinitrofluoren-9-one (1:1) 20265-12-7,
Fluoren-9-one, 2,4,7-trinitro-, compound with naphthalene(1:1)
20265-14-9, Stilbene, compound with 2,4,7-trinitrofluoren-9-one (1:2)
20265-14-9, Fluoren-9-one, 2,4,7-trinitro-, compound with stilbene
(1:1) 25105-01-5, Fluorene, compound with 2,4,7-trinitrofluoren-9-
one 25105-03-7, Phenanthrene, compound with 2,4,7-trinitrofluoren-9-
one 25158-59-2, 11H-Benzo[a]fluorene, compound with
2,4,7-trinitrofluoren-9-one 26104-00-7, Phloroglucinol, isopentyl-
33733-07-2, m-Terphenyl, 5'-methyl- 34379-49-2, 2,4-Xylenol,
6-isobornyl- 35770-75-3, m-Cresol, 4-(α-methylbenzyl)-
40358-51-8, Naphthalene, 1-(1-cyclohexen-1-yl)- 52898-84-7,
Anthracene, compound with 2,4,7-trinitrofluoren-9-one 54986-62-8,
Chrysene, 5-ethyl- 65945-06-4, 2-Chrysenol 66591-49-9, Picene,
compound with 2,4,7-trinitrofluoren-9-one 66591-49-9, Fluoren-9-one,
2,4,7-trinitro-, compound with picene (1:1) 66591-51-3,
11H-Benzo[b]fluorene, compound with 2,4,7-trinitrofluoren-9-one
66591-73-9, Chrysene, 5-ethyl-, compound with 2,4,7-trinitrofluoren-9-
one 66591-74-0, Chrysene, 5-methyl-, compound with
2,4,7-trinitrofluoren-9-one 66591-75-1, Fluoren-9-one,
2,4,7-trinitro-, compound with 1,2,3,4-tetrahydroanthracene (1:1)
66591-76-2, Picene, 5-methyl-, compound with 2,4,7-trinitrofluoren-9-
one 66591-76-2, Fluoren-9-one, 2,4,7-trinitro-, compound with
5-methylpicene (1:1) 66778-03-8, Pyrene, 4-ethyl- 66778-18-5,
1,1'-Binaphthyl, 2,2',7,7'-tetramethyl- 66778-23-2, Bicyclopentyl,
2,2'-dimethyl- 66778-24-3, Naphthalene, 2-o-tolyl 66778-25-4,
Picene, 13-methyl- 66903-94-4, Diindeno[1,2,3-cd:1',2',3'-
lm]perylene, compound with 2,4,7-trinitrofluoren-9-one 66907-64-0,
4H-Cyclopenta[def]phenanthrene, compound with 2,4,7-trinitrofluoren-9-
one (1:1) 66923-92-0, Phenanthrene, 2-phenyl-, compound with
2,4,7-trinitrofluoren-9-one 66923-92-0, Fluoren-9-one,
2,4,7-trinitro-, compound with 2-phenylphenanthrene (1:1)
66923-93-1, Fluoren-9-one, 2,4,7-trinitro-, compound with
1,2,3,4-tetrahydrophenanthrene (1:1) 66923-93-1, Phenanthrene,
1,2,3,4-tetrahydro-, compound with 2,4,7-trinitrofluoren-9-one
66923-94-2, Fluoren-9-one, 2,4,7-trinitro-, compound with
2-methylnaphthalene(2:1) 66923-95-3, 1,2'-Binaphthyl, compound with

2,4,7-trinitrofluoren-9-one 66923-96-4, Chrysene, 5,6-dimethyl-, compound with 2,4,7-trinitrofluoren-9-one 66923-98-6, Chrysene, 6-ethyl-, compound with 2,4,7-trinitrofluoren-9-one 66923-99-7, Pyrene, 4,9-dimethyl-, compound with 2,4,7-trinitrofluoren-9-one 66923-99-7, Fluoren-9-one, 2,4,7-trinitro-, compound with 4,9-dimethylpyrene (1:1) 66924-00-3, Cholanthrene, compound with 2,4,7-trinitrofluoren-9-one 66924-02-5, 1,2'-Binaphthyl, 1'-methyl-, compound with 2,4,7-trinitrofluoren-9-one 66924-03-6, Fluoren-9-one, 2,4,7-trinitro-, compound with 4-ethylpyrene (1:1) 66924-03-6, Pyrene, 4-ethyl-, compound with 2,4,7-trinitrofluoren-9-one 66924-04-7, Chrysene, 6-methyl-, compound with 2,4,7-trinitrofluoren-9-one 66924-05-8, Cholanthrene, 3-methyl-, compound with 2,4,7-trinitrofluoren-9-one 66924-06-9, Fluoren-9-one, 2,4,7-trinitro-, compound with acenaphthene 66924-07-0, Fluoren-9-one, 2,4,7-trinitro-, compound with 1-methylnaphthalene (1:1) 66924-08-1, Phenanthrene, 9-methyl-, compound with 2,4,7-trinitrofluoren-9-one 66924-08-1, Fluoren-9-one, 2,4,7-trinitro-, compound with 9-methylphenanthrene (1:1) 66924-09-2, 7H-Benzo[c]fluorene, compound with 2,4,7-trinitrofluoren-9-one 66924-10-5, Fluoren-9-one, 2,4,7-trinitro-, compound with 4-methylpyrene (1:1) 66924-10-5, Pyrene, 4-methyl-, compound with 2,4,7-trinitrofluoren-9-one 66924-11-6, Fluoren-9-one, 2,4,7-trinitro-, compound with 2-benzylnaphthalene 66924-12-7, Fluoren-9-one, 2,4,7-trinitro-, compound with 2-phenylnaphthalene (1:1) 66924-13-8, Fluoranthene, compound with 2,4,7-trinitrofluoren-9-one (1:1) 66924-14-9, Fluoren-9-one, 2,4,7-trinitro-, compound with diphenylacetylene(1:1) 67011-59-0, Methanol, diphenyl(3,4,5-trihydroxyphenyl)- 90116-17-9, Fluoren-9-one, 2,4,7-trinitro-, compound with 11H-indeno[2,1-a]phenanthrene (1:1) 90914-84-4, Imidazole, 2-(α-aminobenzyl)- 92348-31-7, Cyclohexadienediol, dimethyl- **96674-12-3**, Dibenzo[def,mno]chrysene, compound with 2,4,7-trinitrofluoren-9-one (1:1) 96872-57-0, Fluoren-9-one, 2,4,7-trinitro-, compound with 1,4-diphenyl-1,3-butadiene(2:1) 97331-47-0, Fluoranthene, sodium complex 102217-61-8, Benzidine, diphenyl- 106304-19-2, Benzo[k]fluoranthene, compound with 2,4,7-trinitrofluoren-9-one 106844-42-2, Fluoren-9-one, 2,4,7-trinitro-, compound with 5,6-dihydro-4H-benz[de]anthracene 119925-41-6, Naphthalene, 2-methyl-, compound with 2,4,7-trinitrofluoren-9-one 137065-33-9, 1,3-Butadiene, 1,4-diphenyl-, compound with 2,4,7-trinitrofluoren-9-one

(x-ray diffraction pattern for)

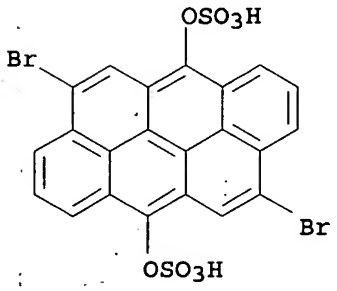
L33 ANSWER 63 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1964:48866 Document No. 60:48866 Original Reference No. 60:8610b-c Chromatography of lactic acid and some other organic carboxylic acids on cellulose. Schweiger, A. (Bundesanstalt Fleischforsch., Kulmbach, Germany). Zeitschrift fuer Lebensmittel-Untersuchung und -Forschung, 124(1), 20-2 (Unavailable) 1963. CODEN: ZLUFAR. ISSN: 0044-3026.

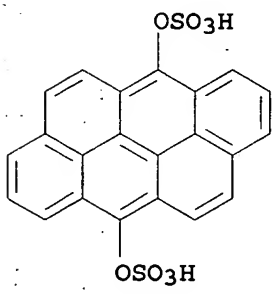
AB On a thin film of cellulose powder, a solvent system of pentanol:HCOOH:H2O (20:20:1) and identification with 0.05% of 8-quinolinol permitted detection of 0.5-1.0 γ of various organic acids. The acids studied, with their RA values (migration in relation to that of malic acid) were: lactic 1.61, malic 1.00, tartaric 0.66, citric 0.75, α-ketoglutaric 1.27, gluconic 0.67, ascorbic 0.77, malonic 1.29, succinic 1.45, glutaric 1.63, adipic 1.77.

IT **4378-58-9**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) **30756-44-6**,

Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate)
(chromatography of)
RN 4378-58-9 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) (8CI, 9CI) (CA INDEX NAME)



RN 30756-44-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate) (9CI) (CA INDEX NAME)

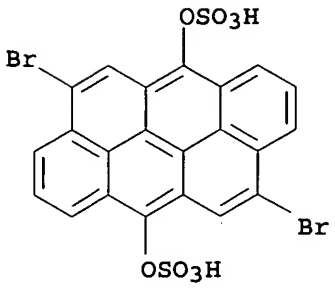


2 (D1—O—Me)

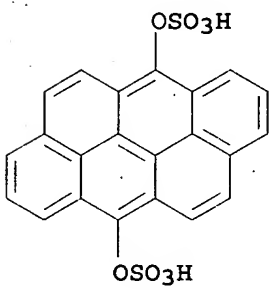
CC 2 (Analytical Chemistry)
IT 50-21-5, Lactic acid 50-81-7, Ascorbic acid 87-69-4, Tartaric acid 110-15-6, Succinic acid 110-94-1, Glutaric acid 124-04-9, Adipic acid 141-82-2, Malonic acid 328-50-7, Glutaric acid, 2-oxo- 2678-71-9, Dinaphtho[1,2,3-cd:3',2',1'-lm]perylene-5,10-diol, 16,17-dimethoxy-, bis(hydrogen sulfate) 3564-70-3, Dibenzo[b,def]chrysen-7,14-ylene sodium sulfate 3687-66-9, Indol-3-ol, 5,7-dichloro-2-(5,6,7-trichloro-3-hydroxy-benzo[b]thien-2-yl)-, bis(hydrogen sulfate) (ester) 4335-00-6, Indol-3-ol, 5-bromo-2-(9-chloro-3-hydroxynaphtho-[1,2-b]thien-2-yl)-, bis(hydrogen sulfate) (ester) **4378-58-9**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) 4388-08-3, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6-chloro-6'-methoxy-4-methyl-, bis(hydrogen sulfate) 4388-09-4, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 5,5'-dichloro-7,7'-dimethyl-, bis(hydrogen sulfate) 4388-10-7, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6,6'-dichloro-4,4'-dimethyl-, bis(hydrogen sulfate) 4388-11-8, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6,6'-diethoxy-, bis(hydrogen sulfate) 4388-12-9, [2,2'-Bibenzo[b]thiophene]-3,3'-

diol, 5,6',7-trichloro-4,4'-dimethyl-, bis(hydrogen sulfate) 4425-36-9, [2,2'-Binaphtho[2,1-b]thiophene]-1,1'-diyl sodium sulfate 5632-11-1, Hydroquinone, 2,5-bis(p-chloroanilino)-, bis(hydrogen sulfate (ester) 6371-40-0, [2,2'-Biindole]-3,3'-diol, 5,6',7-trichloro-, bis(hydrogen sulfate) (ester) 6406-11-7, Indol-3-ol, 5,7-dichloro-2-(6-chloro-3-hydroxy-4-methylbenzo[b]thien-2-yl)-, bis(hydrogen sulfate) (ester) 6527-57-7, 4-Biphenylcarboxamide, N-(9,10-dihydroxy-1-anthryl)-, bis(hydrogen sulfate) 6536-59-0, Indol-3-ol, 5-chloro-2-(4-chloro-1-hydroxy-2-naphthyl)-7-methoxy-4-methyl-, bis(hydrogen sulfate) (ester) 6536-62-5, Indol-3-ol, 5,7-dibromo-2-(1-hydroxy-2-anthryl)-, bis(hydrogen sulfate) (ester) 6897-40-1, 5,9,14,18-Anthrazinetetrol, 7,16-dichloro-6,15-dihydro-, tetrakis(hydrogen sulfate) (ester) 6915-15-7, Malic acid 10127-01-2, [2,2'-Binaphtho[2,3-b]thiophene]-3,3'-diol, 9,9'-dichloro-, bis(hydrogen sulfate), di-Na salt 10380-32-2, [2,2'-Biindole]-3,3'-diol, 4,4',5,5',7,7'-hexabromo-, bis(hydrogen sulfate) (ester), di-Na salt 14933-21-2, Gluconic acid, calcium salt 25044-13-7, Anthra[2,1,9-mna]naphth[2,3-h]acridin-5(16H)-one, 10,15-dihydroxy-, bis(hydrogen sulfate)(ester) 25740-96-9, [2,2'-Biindole]-3,3'-diol, 5-bromo-, bis(hydrogen sulfate) (ester) 25740-98-1, [2,2'-Biindole]-3,3'-diol, 5,5',7,7'-tetrabromo-, bis(hydrogen sulfate) (ester) 27758-22-1, 1,6-Pyrenediol, 5,10-dianilino-3,8-dichloro-, bis(hydrogen sulfate) (ester) **30756-44-6**, Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate) 32033-20-8, Dinaphtho[1,2,3-cd:1',2',3'-lm]perylene-9,18-diol, dichloro-, bis(hydrogen sulfate) 32073-36-2, Dinaphtho[1,2,3-cd:3',2',1'-lm]perylene-5,10-diol, dibromo-16,17-dimethoxy-, bis(hydrogen sulfate) 89232-88-2, Dibenzo[b,def]chrysene-6,12-diol, dibromo-, bis(hydrogen sulfate) 121991-36-4, Benzamide, N,N'-(9,10-dihydroxy-1,5-anthrylene)bis-, bis(hydrogen sulfate)
(chromatography of)

L33 ANSWER 64 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1964:48865 Document No. 60:48865 Original Reference No. 60:8610b
Paper chromatography of dyes. III. Paper chromatography of solubilized vat dyes. Sramek, Jiri (Res. Inst. Textile Finishing, Dvur Kravlove nad Labem, Czech.). Journal of Chromatography, 12(4), 453-63 (Unavailable) 1963. CODEN: JOCRAM. ISSN: 0021-9673.
AB cf. CA 60, 2309h. The descending technique and centrifugal chromatography have good agreement for the separation of solubilized vat dyes by paper chromatography. The principal solvent system used was NH4OH (25%)-MeOH-H2O (1:2:3), but C5H5N-isoamyl alc.-NH4OH (25%) (1.3:1:1) and MeOH-HOAc-H2O (4:1:1) were also applied. Dyes with a simple structure had the highest Rf values, and these increased with increasing size of the mol.
IT **4378-58-9**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) **30756-44-6**, Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate)
(chromatography of)
RN 4378-58-9 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) (8CI, 9CI) (CA INDEX NAME)



RN 30756-44-6 HCAPLUS
CN Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate) (9CI) (CA INDEX NAME)



2 (D1—O—Me)

CC 2 (Analytical Chemistry)
IT 2678-71-9, Dinaphtho[1,2,3-cd:3',2',1'-lm]perylene-5,10-diol, 16,17-dimethoxy-, bis(hydrogen sulfate) 3564-70-3, Dibenzo[b,def]chrysen-7,14-ylene sodium sulfate 3687-66-9, Indol-3-ol, 5,7-dichloro-2-(5,6,7-trichloro-3-hydroxy-benzo[b]thien-2-yl)-, bis(hydrogen sulfate) (ester) 4335-00-6, Indol-3-ol, 5-bromo-2-(9-chloro-3-hydroxynaphtho-[1,2-b]thien-2-yl)-, bis(hydrogen sulfate) (ester) **4378-58-9**, Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) 4388-08-3, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6-chloro-6'-methoxy-4-methyl-, bis(hydrogen sulfate) 4388-09-4, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 5,5'-dichloro-7,7'-dimethyl-, bis(hydrogen sulfate) 4388-10-7, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6,6'-dichloro-4,4'-dimethyl-, bis(hydrogen sulfate) 4388-11-8, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 6,6'-diethoxy-, bis(hydrogen sulfate) 4388-12-9, [2,2'-Bibenzo[b]thiophene]-3,3'-diol, 5,6',7-trichloro-4,4'-dimethyl-, bis(hydrogen sulfate) 4425-36-9, [2,2'-Binaphtho[2,1-b]thiophene]-1,1'-diyl sodium sulfate 5632-11-1, Hydroquinone, 2,5-bis(p-chloroanilino)-, bis(hydrogen sulfate (ester) 6371-40-0, [2,2'-Biindole]-3,3'-diol, 5,6',7-trichloro-, bis(hydrogen sulfate) (ester) 6406-11-7, Indol-3-ol, 5,7-dichloro-2-(6-chloro-3-hydroxy-4-methylbenzo[b]thien-2-yl)-, bis(hydrogen sulfate) (ester) 6527-57-7, 4-Biphenylcarboxamide, N-(9,10-dihydroxy-1-anthryl)-, bis(hydrogen sulfate) 6536-59-0, Indol-3-ol, 5-chloro-2-(4-chloro-1-hydroxy-2-naphthyl)-7-methoxy-4-methyl-, bis(hydrogen sulfate) (ester)

6536-62-5, Indol-3-ol, 5,7-dibromo-2-(1-hydroxy-2-anthryl)-, bis(hydrogen sulfate) (ester) 6897-40-1, 5,9,14,18-Anthrazinetetrol, 7,16-dichloro-6,15-dihydro-, tetrakis(hydrogen sulfate) (ester) 10127-01-2, [2,2'-Binaphtho[2,3-b]thiophene]-3,3'-diol, 9,9'-dichloro-, bis(hydrogen sulfate), di-Na salt 10380-32-2, [2,2'-Biindole]-3,3'-diol, 4,4',5,5',7,7'-hexabromo-, bis(hydrogen sulfate) (ester), di-Na salt 25044-13-7, Anthra[2,1,9-mna]naphth[2,3-h]acridin-5(16H)-one, 10,15-dihydroxy-, bis(hydrogen sulfate)(ester) 25740-96-9, [2,2'-Biindole]-3,3'-diol, 5-bromo-, bis(hydrogen sulfate) (ester) 25740-98-1, [2,2'-Biindole]-3,3'-diol, 5,5',7,7'-tetrabromo-, bis(hydrogen sulfate) (ester) 27758-22-1, 1,6-Pyrenediol, 5,10-dianilino-3,8-dichloro-, bis(hydrogen sulfate) (ester) **30756-44-6**, Dibenzo[def,mno]chrysene-6,12-diol, dimethoxy-, bis(hydrogen sulfate) 32033-20-8, Dinaphtho[1,2,3-cd:1',2',3'-lm]perylene-9,18-diol, dichloro-, bis(hydrogen sulfate) 32073-36-2, Dinaphtho[1,2,3-cd:3',2',1'-lm]perylene-5,10-diol, dibromo-16,17-dimethoxy-, bis(hydrogen sulfate) 89232-88-2, Dibenzo[b,def]chrysene-6,12-diol, dibromo-, bis(hydrogen sulfate) 121991-36-4, Benzamide, N,N'-(9,10-dihydroxy-1,5-anthrylene)bis-, bis(hydrogen sulfate)
(chromatography of)

L33 ANSWER 65 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1962:480505 Document No. 57:80505 Original Reference No. 57:15996g-i
Absorption spectra of the molecular complexes of aromatic compounds with p-bromanil. Kinoshita, Minoru (Tokyo Univ.). Bulletin of the Chemical Society of Japan, 35(No. 9), 1609-11 (Unavailable) 1962. CODEN: BCSJA8. ISSN: 0009-2673.

AB The maximum of the spectra in CCl_4 of complexes of aromatic hydrocarbons and amines with p-bromanil are determined, and used to estimate the ionization potentials (Ip) of several donors by use of the Mulliken charge transfer theory (CA 47, 2596a). The compds., maximum (mμ), and Ip (e.v.) are: naphthalene, 486, 8.08; anthracene, 630, 7.40; phenanthrene, 465, 8.22; pyrene, 608, 7.48; chrysene, 562, 7.68; triphenylene, 487, 8.08; 1,2-benzanthracene 587, 7.56, perylene, 738, 7.06; anthranthrene, 756, 7.01; 1-methylnaphthalene, 418 (503), 7.98; acenaphthene, 566, 7.66; di-Ph, 410, 8.64; p-xylene, 424, 8.52; mesitylene, 421, 8.55; aniline, 560, 7.68; dimethylaniline, 657, 7.31; pchloroaniline, 500, 8.00; o-phenylenediamine, 638, 7.36; diphenylamine, 655, 7.31; phenyl-α-naphthylamine, 718, 7.12; phenyl-β-naphthylamine, 706, 715; α-naphthylamine, 632, 7.39; p-toluidine, 586, 7.58; o-toluidine, 558, 7.69; phenothiazine, 665 (>800), 7.28; acridine, 493, 8.04.

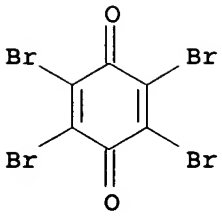
IT **96976-90-8**, p-Benzoquinone, tetrabromo-, compound with dibenzo[def,mno]chrysene (1:1)
(ionization energy and spectrum of)

RN 96976-90-8 HCAPLUS

CN p-Benzoquinone, tetrabromo-, compd. with dibenzo[def,mno]chrysene (7CI) (CA INDEX NAME)

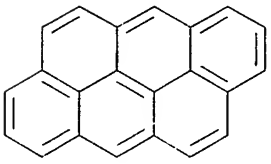
CM 1

CRN 488-48-2
CMF C6 Br4 O2



CM 2

CRN 191-26-4
CMF C22 H12



CC 10 (Spectra and Some Other Optical Properties)
IT 1939-57-7, p-Benzoquinone, tetrabromo-, compound with pyrene (1:1)
14147-73-0, Anthracene, compound with tetrabromo-p-benzoquinone
16541-29-0, p-Benzoquinone, tetrabromo-, compound with naphthalene (1:1) 16541-30-3, p-Benzoquinone, tetrabromo-, compound with phenanthrene (1:1) 22011-63-8, Aniline, N,N-dimethyl-, compound with tetrabromo-p-benzoquinone (1:1) 22134-86-7, p-Benzoquinone, tetrabromo-, compound with 1-naphthylamine (1:1) 50849-12-2, p-Benzoquinone, tetrabromo-, compound with perylene (1:1)
55677-21-9, p-Benzoquinone, tetrabromo-, compound with phenothiazine (1:1) 57431-87-5, p-Benzoquinone, tetrabromo-, compound with biphenyl (1:1) 57431-88-6, p-Benzoquinone, tetrabromo-, compound with triphenylene (1:1) 61755-80-4, Acenaphthene, compound with tetrabromo-p-benzoquinone 88644-88-6, p-Benzoquinone, tetrabromo-, compound with chrysene (1:1) 88842-72-2, Benz[a]anthracene, compound with tetrabromo-p-bromoquinone (1:1) 91371-19-6, Aniline, p-chloro-, compound with tetrabromo-p-benzoquinone (1:1) 93191-72-1, p-Benzoquinone, tetrabromo-, compound with 1-methylnaphthalene (1:1)
94375-70-9, Acridine, compound with tetrabromo-p-benzoquinone
94502-80-4, Aniline, compound with tetrabromo-p-benzoquinone (1:1)
95467-97-3, p-Benzoquinone, tetrabromo-, compound with o-phenylenediamine (1:1) 96313-39-2, p-Benzoquinone, tetrabromo-, compound with o-toluidine (1:1) 96313-40-5, p-Benzoquinone, tetrabromo-, compound with p-toluidine (1:1) **96976-90-8**, p-Benzoquinone, tetrabromo-, compound with dibenzo[def,mno]chrysene (1:1) 96983-48-1, p-Benzoquinone, tetrabromo-, compound with p-xylene (1:1) 97340-22-2, p-Benzoquinone, tetrabromo-, compound with mesitylene (1:1) 98146-91-9, p-Benzoquinone, tetrabromo-, compound with Ph2NH (1:1) 106458-71-3, p-Benzoquinone, tetrabromo-, compound with N-phenyl-1-naphthylamine (1:1) 561024-22-4, p-Benzoquinone, tetrabromo-, compound with N-phenyl-2-naphthylamine (1:1)
(ionization energy and spectrum of)

L33 ANSWER 66 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1962:480261 Document No. 57:80261 Original Reference No. 57:15954d-f
Semiconductivities and charge transfer spectra of solid molecular complexes of 1,3,5-trinitrobenzene. Kuroda, Haruo; Yoshihara, Keitaro; Akamatsu, Hideo (Tokyo Univ.). Bulletin of the Chemical Society of Japan, 35, 1604-8 (Unavailable) 1962. CODEN: BCSJA8. ISSN: 0009-2673.

AB A series of solid complexes of aromatic hydrocarbons and amines with 1,3,5-trinitrobenzene as the common electron acceptor were prepared These complexes were of the loose mol. complex type, and the charge transfer bands were observed with the solid complexes, which showed only small red-shifts from the corresponding bands of the solns. These solid complexes are poor semiconductors. The energy gap for the excitation to the conduction state is relatively large and is nearly coincident with the energy for the charge transfer excitation. Apparently the charge transfer state in the crystal may not differ much from the corresponding state in the isolated (1:1) complex in the solution The relation between the charge-transfer state and the conduction state is discussed, and a probable model for the formation of a charge carrier is suggested.

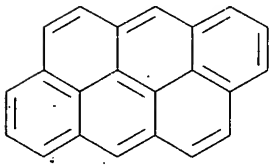
IT **34892-84-7**, Dibenzo[def,mno]chrysene, compound with 1,3,5-trinitrobenzene
(elec. semicond. and spectrum of)

RN 34892-84-7 HCAPLUS

CN Dibenzo[def,mno]chrysene, compd. with 1,3,5-trinitrobenzene (1:1) (9CI) (CA INDEX NAME)

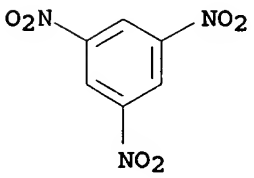
CM 1

CRN 191-26-4
CMF C22 H12



CM 2

CRN 99-35-4
CMF C6 H3 N3 O6

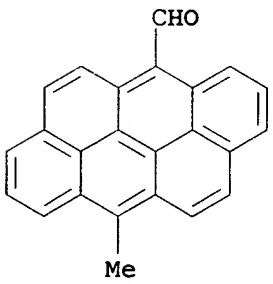


CC 9 (Electric and Magnetic Phenomena)

IT 2499-09-4, Anthracene, compound with 1,3,5-trinitrobenzene
6164-86-9, Pyrene, compound with 1,3,5-trinitrobenzene (1:1)
16580-43-1, Aniline, compound with 1,3,5-trinitrobenzene 16615-54-6,

Aniline, p-chloro-, compound with 1,3,5-trinitrobenzene 16615-59-1, p-Phenylenediamine, compound with 1,3,5-trinitrobenzene 16636-09-2, Aniline, N,N-dimethyl-, compound with 1,3,5-trinitrobenzene 16636-10-5, 1-Naphthylamine, compound with 1,3,5-trinitrobenzene 20265-09-2, Benzidine, compound with 1,3,5-trinitrobenzene 23950-31-4, Perylene, compound with 1,3,5-trinitrobenzene 29271-85-0, Phenanthrene, compound with 1,3,5-trinitrobenzene **34892-84-7**, Dibenzo[def,mno]chrysene, compound with 1,3,5-trinitrobenzene 72735-57-0, Chrysene, compound with 1,3,5-trinitrobenzene 95131-55-8, Benzidine, N,N,N',N'-tetramethyl-, compound with 1,3,5-trinitrobenzene 105819-69-0, Violanthrene, compound with 1,3,5-trinitrobenzene
(elec. semicond. and spectrum of)

L33 ANSWER 67 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1962:4378 Document No. 56:4378 Original Reference No. 56:839e-f The carcinogenic activity of aldehyde derivatives of anthracene and of 3,4,8,9 and 3,4,9,10-dibenzopyrenes. Lacassagne, Antoine; Buu-Hoi, Ng. Ph.; Zajdela, Francois; Lavit-Lamy, Denise Compt. Rend., 252, 1711-13 (Unavailable) 1961.
AB The aldehyde derivatives, 6-formylanthracene, 6-formyl, 12-methylanthracene, 5-formyl-8-methyl-3,4,9,10-dibenzopyrene, 5-formyl-3,4,8,9-dibenzopyrene, and 5-formyl-3,4,9,10 dibenzopyrene are strongly carcinogenic in the XVII nc/Z strain of mice.
IT **63040-58-4**, Dibenzo[def,mno]ohrysene-6-carboxaldehyde, 12-methyl-
(carcinogenicity of)
RN 63040-58-4 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-carboxaldehyde, 12-methyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 71 (Mammalian Pathological Chemistry)
IT 63040-53-9, Benzo[rst]pentaphene-5-carboxaldehyde 63040-54-0, Dibenzo[b,def]chrysene-7-carboxaldehyde 63040-56-2, Benzo[rst]pentaphene-5-carboxaldehyde, 8-methyl- 63040-57-3, Dibenzo[b,def]chrysene-7-carboxaldehyde, 14-methyl- **63040-58-4**, Dibenzo[def,mno]ohrysene-6-carboxaldehyde, 12-methyl-
(carcinogenicity of)

L33 ANSWER 68 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1960:56366 Document No. 54:56366 Original Reference No. 54:10983b-i,10984a-b Azulene. VIII. A study of the visible absorption spectra and dipole moments of some 1- and 1,3-substituted azulenes. Anderson, Arthur G., Jr.; Steckler, Bernard M. (Univ. of Washington, Seattle). Journal of the American Chemical Society, 81, 4941-6 (Unavailable) 1959. CODEN: JACSAT. ISSN: 0002-7863.

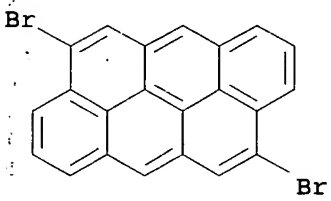
AB cf. C.A. 54, 4525c; Cowles, C.A. 51, 7144g. Solution dipole moments and visible absorption spectra were determined for the following compds. (D. and λ given): azulene (I), 1.08, 580; 1,3-dichloroazulene (II), 2.45, 638; 1,3-dibromoazulene (III), 2.52, 625; 1,3-diiodoazulene (IV), 2.42, 616; 1-nitroazulene (V), 6.06, 532 mμ. I, m. 100-100.5° (hexane), was prepared by a modified Ziegler-Hafner method. II, deep green needles, m. 90.0-90.5° (hexane), III, m. 90.5-1.5° (hexane), and V, tiny deep red needles, m. 109-10° (hexane and CH_2Cl_2-petr. ether), were prepared as described previously. IV, deep blue-green feathery needles, amorphous above 100° (C_6H_6), was prepared in 90% yield from 3.02 g. N-iodosuccinimide (VI), 0.853 g. I, and 65 ml. dry CH_2Cl_2, stirred 10 hrs., and chromatographed, λ (log ε) 243 (1.35), 278 (1.21), 309 (1.73), 337 (0.18), 344 (0.24), 350 (0.28), 359 (0.41), 368 (0.26), 376 (0.54), 616 (1.25), 674 (1.1), and 752 mμ (0.42). 1-Chloro-3-phenylazoazulene (VII), fluffy green needles, m. 115-16° (cyclohexane), λ (log ε) 239 (4.36), 282 (4.32), 331 (4.27), 426 (4.46), and 634 mμ (ε 655), was prepared in 49% yield by refluxing 70 mg. 1-phenylazoazulene (VIII), 40 mg. N-chlorosuccinimide, and 6 ml. dry C_6H_6 11 hrs. and chromatographing the residue. VII was also prepared in 54% yield by the reaction of 1-chloroazulene and benzenediazonium chloride (IX). 1-Bromo-3-phenylazoazulene (X), green-black needles, m. 114-15° (petr. ether), λ (log ε) 238 (4.38), 284 (4.34), 331 (4.28), 427 (4.44), and 619 mμ (ε 641), was prepared in 65% yield by the reaction of 25 mg. VIII in 2 ml. dry C_6H_6 with 19.3 mg. N-bromosuccinimide (XI) at room temperature overnight, followed by another portion of XI, keeping 1 hr., and finally chromatographing. 1-Iodo-3-phenylazoazulene, turquoise plates, m. 148.5-9.5° (cyclohexane), λ (log ε) 245 (4.45), 284 (4.42), 335 (4.33), 428 (4.45), and 626 mμ (ε 648), was prepared in 75% yield by the reaction of 50 mg. VIII with 48.5 mg. VI in 5 ml. C_6H_6, 11 days after which another portion of VI was added, and the mixture allowed to stand 2 days before chromatographing. 1-Nitro-3-phenylazoazulene, shiny, black needles, m. 153.5-4.5° (CH_2Cl_2-petr. ether), λ (log ε) 240 (4.32), 322 (4.36), 399 (4.48), and 5.62 mμ (ε 1037), was prepared in 11% yield from 250 mg. VIII, 35 ml. Ac_2O, and 1.2 ml. M HNO_3 in Ac_2O, stirred 35 hrs., and chromatographed. 1-Methyl-3-phenylazoazulene (XII), viscous dark brown oil which solidified after several weeks, m. 38-48°, λ (log ε) 243 (4.31), 282 (4.29), 337 (4.21), 432 (4.43), 582 (ε 516), 612 (ε 511), and 633 mμ (ε 508), was prepared in 79% yield from the reaction of IX with 116 mg. 1-methylazulene and 400 mg. AcONa in 8 ml. EtOH followed by chromatography of the residue. IX was freshly prepared at 0° from 108 mg. anilinium chloride, 0.2 ml. concentrated HCl, and 57 mg. $NaNO_2$ in 2 ml. H_2O. The chromatographic adsorption treatment was described for each preparation Spectra were taken in cyclohexane, except that of X in hexane. A trinitrobenzene derivative of XII, tiny fluffy black needles, m. 163.5-4.5°, was prepared in 54% yield. Rough energy diagrams were given for the substituents studied to show splitting and stabilization. Dipole moments in each case showed that the direction of the group moment axis was from the nucleus to the substituent. Halo, PhN: N, MeC(: NOH), and similar groups stabilized the excited state through a mesomeric electron release to a greater extent than the azulene nucleus stabilized the ground state through an inductive electron release. Nitro group stabilized the ground state through both resonance and inductive mechanisms but had little or no ability to stabilize the excited

state so that increased excitation energy resulted. For alkyl groups, the stabilization of the excited state through inductive and(or) hyperconjugative mechanisms far exceeded any change in the ground state. Ph stabilized both states but with greater effect on the excited state. The foregoing reasoning explained the unexpected red spectral shift for the nitro group and the blue shift for the halo group. In the spectrum of VIII in hexane, a band at 416 mμ was similar to that of azobenzene, λ 420 mμ (EtOH), and thus was assigned to the azoaromatic linkage. The 609 mμ band, shifted +29 mμ, was attributed to the PhN:N group on the 1-position of azulene. The nucleus component of a halogen substituted azulene could be assumed to be the same as in azulene. The calculated moments for C-Cl, C-Br, and C-I were 2.2, 2.3, and 2.2 D., resp.

IT **102442-54-6**, Dibenzo[def,mno]chrysene, 4,10-dibromo-
(preparation of)

RN 102442-54-6 HCAPLUS

CN Dibenzo[def,mno]chrysene, 4,10-dibromo- (6CI) (CA INDEX NAME)



CC 10F (Organic Chemistry: Condensed Carbocyclic Compounds)

IT 16294-32-9, Anthracene, 1,5-dimethoxy- 16294-34-1, Anthracene, 1,8-dimethoxy- **102442-54-6**, Dibenzo[def,mno]chrysene, 4,10-dibromo- 102546-25-8, 1-Azuleneazobenzene, 3-methyl- 102546-26-9, 1-Azuleneazobenzene, 3-methyl-, compound with 1,3,5-trinitrobenzene
(preparation of)

L33 ANSWER 69 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1959:49118 Document No. 53:49118 Original Reference No. 53:8805c-d

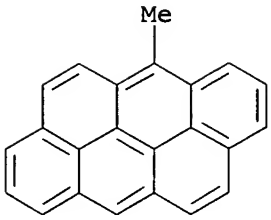
The ultraviolet, visible, and infrared absorption of certain hexacyclic aromatic hydrocarbons and their methylated homologues. Buu-Hoi, Ng. Ph.; Lavit, Denise (Univ. Paris). Bulletin de la Societe Chimique de France 1404-6 (Unavailable) 1958. CODEN: BSCFAS. ISSN: 0037-8968.

AB Ultraviolet, visible, and infrared absorption spectra are reported for anthanthrene (I), its meso-Me and meso-di-Me derivs., di-benzo[a,h]pyrene (II), its meso-Me and meso-di-Me derivs., and for naphtho[2,3-a]pyrene and its 6-Me, 9-Me, and 9,10-di-Me derivs. Introduction of meso-Me groups produces a much more important bathochromic shift in I than in II. A band at about 11.4 μ in I progressively disappears on meso-methylation, and is ascribed to a vibration of meso-H atoms.

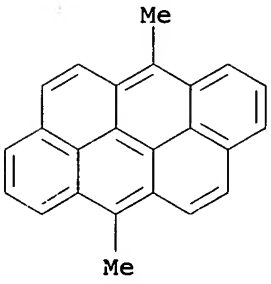
IT **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl-
41217-05-4, Dibenzo[def,mno]chrysene, 6,12-dimethyl-
63040-55-1, Dibenzo[def,mno]chrysene-6-carboxaldehyde
(spectrum of)

RN 31927-64-7 HCAPLUS

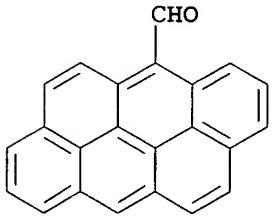
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



RN 63040-55-1 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-carboxaldehyde (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 3 (Electronic Phenomena and Spectra)
IT 189-64-0, Dibenzo[b,def]chrysene 191-26-4, Dibenzo[def,mno]chrysene 196-42-9, Naphtho[2,1,8-qra]naphthacene 5174-22-1, Dibenzo[b,def]chrysene, 7-methyl- 16982-39-1, Naphtho[2,1,8-qra]naphthacene, 9,10-dimethyl- **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl- **41217-05-4**, Dibenzo[def,mno]chrysene, 6,12-dimethyl- **63040-55-1**, Dibenzo[def,mno]chrysene-6-carboxaldehyde 83439-54-7, Dibenzo[b,def]chrysene, 7,14-dimethyl-
(spectrum of)

L33 ANSWER 70 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1959:1885 Document No. 53:1885 Original Reference No. 53:284g-h
Molecular complexes of tetrabromophthalic anhydride. Jacquignon, Pierre; Buu-Hoi, Ng. Ph. (Univ. Paris). Bulletin de la Societe Chimique de France (No. 6), 761-6 (Unavailable) 1958. CODEN: BSCFAS. ISSN: 0037-8968.

AB Tetrabromophthalic anhydride (I) forms heat sensitive, 1:1 complexes with donor electron compds. of varied structures. I, m. 279-80%°, can be prepared in almost quant. yield by heating at 65° 25 g. of C6H4(CO)2O in 150 g. fuming H2SO4 (65% SO3) and 105 g. Br. After 3 hrs. at 170° and then 30 min. at 200° the product is isolated and recrystd. from boiling HOAc.

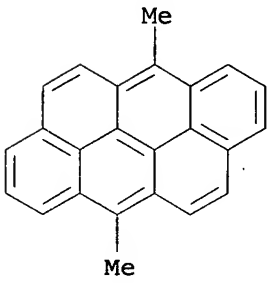
IT **103402-84-2**, Dibenzo[def,mno]chrysene, 6,12-dimethyl-, compound with tetrabromophthalic anhydride
(preparation of)

RN 103402-84-2 HCAPLUS

CN Phthalic anhydride, tetrabromo-, compd. with 6,12-dimethyldibenzo[def,mno]chrysene (6CI) (CA INDEX NAME)

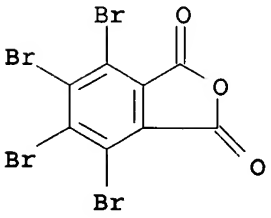
CM 1

CRN 41217-05-4
CMF C24 H16



CM 2

CRN 632-79-1
CMF C8 Br4 O3



CC 10E (Organic Chemistry: Benzene Derivatives)

IT 59005-66-2, Benzene, hexamethyl-, compound with tetrabromophthalic anhydride 72616-99-0, Fluoranthene, compound with tetrabromophthalic anhydride 72617-00-6, Naphthalene, 2-methyl-, compound with tetrabromophthalic anhydride 102159-73-9, Carbazole, 1,2,3,4-tetrahydro-, compound with tetrabromophthalic anhydride 102184-34-9, Naphthalene, 2,7-dimethyl-, compound with tetrabromophthalic anhydride 102184-35-0, Naphthalene, 1,5-dimethoxy-, compound with tetrabromophthalic anhydride 102442-96-6, 1-Naphthaldehyde, 4-methoxy-5,8-dimethyl-, compound with tetrabromophthalic anhydride 102947-72-8, Naphthalene, 2,6-di-tert-butyl-, compound with tetrabromophthalic anhydride

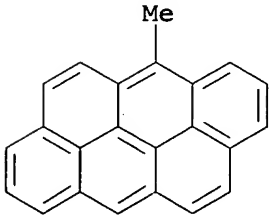
103402-84-2, Dibenzo[def,mno]chrysene, 6,12-dimethyl-, compound with tetrabromophthalic anhydride 103569-00-2, Pyrene, 1-chloro-, compound with tetrabromophthalic anhydride 110662-73-2, Naphthalene, 6-ethyl-2,3-dimethoxy-, compound with tetrabromophthalic anhydride 113687-51-7, 1-Cyclohexene-1-carboxylic acid, 2-(1,8-dihydroxy-2-naphthyl)-, δ-lactone, compound with tetrabromophthalic anhydride 114617-21-9, Benzo[a]pyrene, compound with tetrabromophthalic anhydride 114696-27-4, Naphthalene, 4-benzyl-1,5-dimethoxy-, compound with tetrabromophthalic anhydride 114722-39-3, 2-Naphthaleneacrylic acid, 1-hydroxy-8-methoxy-β-methyl-, δ-lactone, compound with tetrabromophthalic anhydride 114984-86-0, 2-Naphthaleneacrylic acid, 1,8-dihydroxy-β-methyl-, δ-lactone, compound with tetrabromophthalic anhydride 121292-42-0, Perylene, compound with tetrabromophthalic anhydride 121292-43-1, Dinaphtho[2,1-b:2',3'-d]furan, compound with tetrabromophthalic anhydride 121543-51-9, Cholanthrene, 3-methyl-, compound with tetrabromophthalic anhydride 121544-28-3, Dibenz[a,j]anthracene, compound with tetrabromophthalic anhydride 121621-25-8, 7H-Benzo[c]carbazole, 3,6-dimethyl-, compound with tetrobromophthalic anhydride 122447-84-1, Benz[e]indeno[1,2-b]indole, 7,12-dihydro-9-methyl-, compound with tetrabromophthalic anhydride 124116-12-7, Cyclopentadec[b]indole, 5,6,7,8,9,10,11,12,13,14,15,16,17,18-tetradecahydro-5-methyl-, compound with tetrabromophthalic anhydride
(preparation of)

L33 ANSWER 71 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1958:67905 Document No. 52:67905 Original Reference No. 52:12220h-i
Relation between molecular structure and carcinogenicity in three series of hexacyclic aromatic hydrocarbons. Lacassagne, Antoine; Buu-Hoi, Nguyen Ph.; Zajdela, Francois Compt. rend., 246, 1477-80 (Unavailable) 1958.

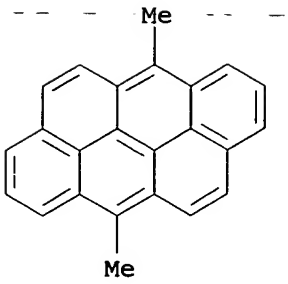
AB A comparative study has been made of the carcinogenicity of 3,4,9,10-dibenzopyrene, 3,4,8,9-dibenzopyrene, anthracene, and the six mono- and dimethyl homologs of 3 hexacyclic hydrocarbons. Meso methylation of the two dibenzopyrenes decreased their activity, while it increased the carcinogenic action of the anthracenes.

IT **31927-64-7**, Dibenzo[def,mno]chrysene, 6-methyl-
41217-05-4, Dibenzo[def,mno]chrysene, 6,12-dimethyl-
(carcinogenic action of)

RN 31927-64-7 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 41217-05-4 HCAPLUS
CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 11H (Biological Chemistry: Pharmacology)
IT 189-55-9, Benzo[rst]pentaphene 189-64-0, Dibenzo[b,def]chrysene
191-26-4, Dibenzo[def,mno]chrysene **31927-64-7**,
Dibenzo[def,mno]chrysene, 6-methyl- 33942-87-9,
Dibenzo[b,def]chrysene, 5-methyl- 33942-88-0,
Benzo[rst]pentaphene, 5-methyl- **41217-05-4**,
Dibenzo[def,mno]chrysene, 6,12-dimethyl- 56309-78-5,
Benzo[rst]pentaphene, 5,8-dimethyl- 122094-93-3,
Dibenzo[b,def]chrysene, 5,10-dimethyl-
(carcinogenic action of)

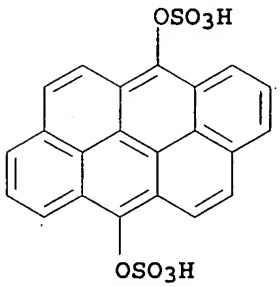
L33 ANSWER 72 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1958:25452 Document No. 52:25452 Original Reference No. 52:4588h-i,4589a-d Sulfuric esters of polycyclic quinols. Bradley, William; Lee, John Gerald (Univ. Leeds, UK). Journal of the Chemical Society, Abstracts 3549-54 (Unavailable) 1957. CODEN: JCSAAZ. ISSN: 0590-9791.
AB To 50 g. C5H5N and 10 g. ClSO3H (mixed below 20°) at 60° was added 6 g. anthraquinone and 4 g. Fe powder, the whole shaken vigorously 3 hrs. at 60-70°, added to 15 g. Na2CO3 in 300 cc. H2O, the whole steam distilled in vacuo, filtered, and the filtrate treated with NaCl to give 11 g. crude di-Na 9,10-anthrylene disulfate (I); the crude I (30 g.) in 150 cc. H2O containing a few drops of aqueous NaOH at 90° with C filtered and the filtrate cooled gave pure I.4H2O, yellow plates; I and dilute HNO3 or NaNO2 gave anthraquinone. I (5 g.) and excess Ba(OAC)2 in H2O gave the Ba salt (II), and II with K2SO4 gave BaSO4 which was filtered off, and the filtrate treated with KCl giving the di K salt-2H2O (III). In similar fashion were prepared di-Na 6,12-anthanthrenylene disulfate (IV) and di-Na 1,2,6,7-dibenzopyren-3,8-ylene disulfate-2H2O (V). p-MeC6H4SO2Cl 1.5 g., 1.0 g. anthrone, and 2.5 cc. C5H5N heated on an H2O bath gave 9-p-toluenesulfonyloxyanthracene (VI), m. 167-8° (alc.). VI (0.4 g.), Raney Ni, and 200 cc. alc. shaken with H overnight gave 10-20% anthracene (VII); under similar conditions, III gave VII, IV gave anthanthrene, and V gave 1,2,6,7-dibenzopyrene. I or III heated rapidly to 90° gave anthraquinol; aeration of I in aqueous NaOH gave naphthadianthrone, 10,10'-dianthronyl, and dianthronol. IV was stable at 90° in air; in the absence of air, the yellow anhydrous salt (VIII) formed; at 160°, VIII decomposed evolving SO2. Anhydrous III refluxed with PhNH2 and HBO3 gave 9,10-dianilinoanthracene, yellow plates, m. 295-300°. V and PhNH2 heated to 150° gave 1,2,6,7-dibenzopyrene-3,8-quinone. III and aqueous KCN heated 3 hrs. at 125° gave anthraquinone and unchanged III; III and NaOEt did not react. The Et3N salt of 10-acetoxy-9-anthryl H sulfate undergoes loss of the Ac group in the presence of aqueous NaOH; under the same conditions III is unaffected. By procedures described above there were obtained di-K p-phenylene

disulfate, m. 287° (H2O), K p-hydroxyphenyl sulfate, m. 220° (alc.) and K Ph sulfate. I with 60% H2O2 and concentrated HCl gave 2-hydroxyanthraquinone and anthraquinone; under similar conditions, IV gave only an unidentified brick-red precipitate

IT **114305-09-8**, Dibenzo[def,mno]chrysen-6,12-ylene sodium sulfate **114305-70-3**, Dibenzo[def,mno]chrysen-6,12-ylene sulfate
(preparation of)

RN 114305-09-8 HCAPLUS

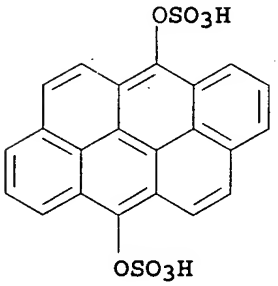
CN Dibenzo[def,mno]chrysen-6,12-ylene sodium sulfate (6CI) (CA INDEX NAME)



●2 Na

RN 114305-70-3 HCAPLUS

CN Dibenzo[def,mno]chrysen-6,12-ylene sulfate (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 128-66-5, Dibenzo[b,def]chrysene-7,14-dione 129-43-1, Anthraquinone, 1-hydroxy- 189-64-0, Dibenzo[b,def]chrysene 191-26-4, Dibenzo[def,mno]chrysene 192-77-8, 9H-Benz[4,5]indeno[2,1-c]phenanthrene 199-94-0, 7H-Benz[de]anthracene 204-56-8, 7H-Benz[4,5]indeno[1,2-a]phenanthrene 434-84-4, 10,10'-Bianthrone 475-64-9, Phenanthro[1,10,9,8-opqra]perylene-7,14-dione 605-32-3, Anthraquinone, 2-hydroxy- 1733-88-6, Phenyl potassium sulfate 2233-88-7, 9,10-Anthracenediamine, N,N'-diphenyl- 3564-70-3, Dibenzo[b,def]chrysen-7,14-ylene sodium sulfate 6252-81-9, Dibenzo[b,def]chrysen-7,14-ylene sulfate 21347-16-0, 9,10-Anthrylene sulfate, (C14H10O2 (SO3)2 102242-35-3, 9-Anthrol, p-toluenesulfonate 110937-95-6, Triethylamine, compound with 9,10-anthradiol sulfate **114305-09-8**, Dibenzo[def,mno]chrysen-6,12-ylene sodium sulfate

114305-70-3, Dibenzo[def,mno]chrysen-6,12-ylene sulfate
116027-33-9, 10,10'-Bianthrone, 10,10'-dihydroxy- 131976-36-8,
7H-Benz[de]anthracene, picrate
(preparation of)

L33 ANSWER 73 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1957:21672 Document No. 51:21672 Original Reference No. 51:4338g-i,4339a-g Electrophilic substitution. V. Competitive nitrations. Dewar, M. J. S.; Mole, T.; Warford, E. W. T. (Queen Mary Coll., London). Journal of the Chemical Society, Abstracts: 3576-80 (Unavailable) 1956. CODEN: JCSAAZ. ISSN: 0590-9791.

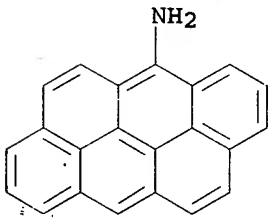
AB Competitive nitrations were carried out in order to determine the reactivities of several unsubstituted poly-cyclic aromatic hydrocarbons relative to one another. The rate constants were calculated by using the formula: k1/k2 = {log10[HC1]0 - log10([HC1]0 - [N1])}/{log10[HC2]0 - log10([HC2]0 - [N2])} (HC1 and HC2 represent the hydrocarbons and N1 and N2 are the corresponding nitro derivs.). The problem resolved itself into one of estimating the amts. of the nitro compds. of each hydrocarbon in the products of the competitive nitrations. In some cases the nitro compds. were separated by chromatography. The following improvement was noted in the Mannich synthesis of triphenylene(I). Cyclohexanone (400 ml.) was condensed and the product poured into H2O, extracted with C6H6, the extract distilled, the fraction b0.3 160° collected, poured into 100 ml. Me2CO, and stirred giving 37 g. dodecahydrotriphenylene (II), m. 180-210°. Dehydrogenation of II by 5% Pd-C at 400°, followed by chromatography gave 65% I, m. 190-4°. The m.p. was raised by decomposition of the recrystd. picrate on Al2O3 to 195.5-6.5°. Estimation of nitrophenanthrene-9-C14 (IIa) were carried out by wet combustion to CO2, which ws counted in a gas-filled Geiger tube. Mononitro derivs. of naphthalene (III), biphenyl (IV), I, chrysene (V), and pyrene (VI) were analyzed in this manner. (a) Fuming HNO3 (0.13 ml.) in 20 ml. ice-cold Ac2O added to a solution of 0.636 g. VI and 8.741 g. III in 300 ml. Ac2O at 0°, solution stirred 2 hrs. at 0°, and left overnight at 2° and the products chromatographed on Al2O3 gave 55.9 mg. nitronaphthalenes (VII) and 99.2 mg. nitropyrene. These wts. led to the value k(HC)/k (III) = 29. In expts. a-e the nitro compds. were separated by chromatography. (b) III (1.781 g.) and V (0.546 g.) similarly treated yielded 0.287 g. nitrochrysenes and 0.363 g. VII. (c) III (13.222 g.) and 0.407 g. benzo[a]pyrene (VIII) similarly treated and purified yielded 0.170 g. VII, 0.177 g. 6-nitrobenzo[a]pyrene, m. 252-4°, and 0.041 g. orange solid, m. 175-210°. (d) Likewise 17.6 g. III and 0.136 g. anthanthrene (IX) gave 35 mg. VII and two nitroanthanthrenes, brown needles (39 mg.) and 34 mg. of a red solid. (e) III (18.052 g.) and 0.972 g. perylene (X) treated as in b gave 0.188 g. VII and 0.750 g. nitroperylene, red crystals, m. 208-10°. (f) C6H6 (169 g.) and 0.876 g. phenanthrene (XI) similarly treated yielded 0.192 g. nitrophenanthrenes (XII) and 0.151 g. PhNO2. (g) Phenanthrene-9-C14 (XIII) (0.955 g.) (17,240 counts min.-1 mg.-1) and 6.293 g. IV similarly nitrated and purified yielded a IIa content of 0.253 g. The mixed nitro compds. weighed 0.331 g. and had a count of 11,150 counts min.-1 mg.-1 (h) XIII (4.784 g.) and 0.398 g. VI likewise gave 0.526 g. of a golden yellow partially crystalline solid having a count of 1802 min. -1 mg.-1, indicating a IIa content of 0.210 g. (i) XIII (1.777 g.) and 0.508 g. V nitrated and chromatographed as in h yielded 0.564 g. of a mixture of nitro compds. which contained 0.287 g. IIa. (j) XIII (2.751 g.) and 0.941 g. I nitrated and the IIa isolated as in g showed a content of 0.550 g. IIa. (k) XIII

(1.061 g.) and 0.980 g. III nitrated and the experiment continued as in g; chromatography 5 times from ligroine containing 10% C6H6 yielded 0.67 g. of mixed nitro compds., whose count indicated a IIa content of 0.372 g. A similar experiment with non-radioactive XI gave VII and XII. The value of k/k1 = 1.4. (l) III (0.956 g.) and 130 g. C6H6 were nitrated and the product prepared as in f and all except 50 ml. distilled through a Dixon gauze column. The residue chromatographed 5 times yielded 0.736 g. of an oil. Comparison with mixture of known materials indicated that the mixture contained 33% PhNO2. (m) III (4.008 g.) and 1.425 g. I nitrated and continued as in g yielded 1.034 g. of mixed nitro compds. and analysis showed a content of 45.8% VII. (n) Coronene (XIV) (0.216 g.) and 0.407 g. III nitrated at 23° in Ac2O and the product chromatographed as before gave no separation of bands. The whole of the band was eluted giving 205 mg. of a yellow residue and analysis indicated that it contained 20% XIV and 80% nitrocoronene (XV). The mixture (80 mg.) was recrystd. to give 40 mg. XV, m. above 360°, ultraviolet absorption values given. The following results were obtained (hydrocarbon, k(HC)/k(X) relative to III, and XI given): C6H6, 0.0025, 0.0026; IV, -, 0.042; VI, 29, 29; I, 4.4, 2.3; V, 4.1, 2.6. Values for k(HC)/k(X) relative to III with the hydrocarbon are: X, 150; VIII, 64; IX, 290; XIV, 6.9.

IT **113951-46-5**, Dibenzo[def,mno]chrysen-6(?)-amine
(preparation of)

RN 113951-46-5 HCAPLUS

CN Dibenzo[def,mno]chrysen-6-amine (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 217-59-4, Triphenylene 63041-90-7, Benzo[a]pyrene, 6-nitro- 68455-92-5, Phenanthrene, nitro- 70021-42-0, Benzo[a]pyrene, nitro- 80182-36-1, Perylene, nitro- 81316-84-9, Coronene, nitro- 98864-46-1, Triphenylene, dodecahydro- **113951-46-5**, Dibenzo[def,mno]chrysen-6(?)-amine
(preparation of)

L33 ANSWER 74 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1957:21671 Document No. 51:21671 Original Reference No. 51:4337i,4338a-g Electrophilic substitution. IV. Nitration of biphenyl. chrysene, benzo[a]-pyrene, and anthanthrene. Dewar, M. J. S.; Mole, T.; Urch, D. S.; Warford, E. W. T. (Queen Mary Coll., London). Journal of the Chemical Society, Abstracts 3572-5 (Unavailable) 1956. CODEN: JCSAAZ. ISSN: 0590-9791.

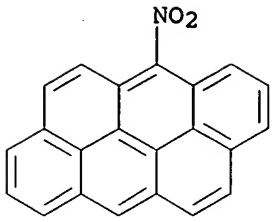
AB Biphenyl (I), chrysene (II), benzo[a]pyrene (III), and anthanthrene (IV) were nitrated by HNO3 in Ac2O. The results were compared with the predictions of a mol.-orbital treatment (C.A. 46, 10715f). The ratio of isomers formed by nitration of I was determined spectrophotometrically. It was established that II and III each yield more than one isomer on nitration. IV gave 2 nitro compds.; x- (V) and y-nitroanthanthrene (VI) were described and their

possible structures were discussed. Anthanthrone, prepared from 1,1'-binaphthyl-8,8'-dicarboxylic acid, was reduced to IV, and purified by chromatography from C6H6. Fuming HNO3 (1.4 ml.) in 20 ml. ice-cold Ac2O was added slowly to 7.7 g. I in 250 ml. Ac2O at 0°, and after 24 hrs. the mixture was hydrolyzed, and the crude residue chromatographed to give 3.07 g. mixed oily nitro compds.; 2.2 g. of this mixture was crystallized from alc. to give 4-nitrobiphenyl (VII), needles, m. 114-15°, and 2-nitrobiphenyl (VIII), prisms, m. 34-6°. From a comparison of the ultraviolet spectrum of the mixture with the spectra of pure VII and VIII, it was concluded that the ratio of VIII to VII was 3.3:1. II (1.2 g.) similarly nitrated and the product chromatographed gave 0.454 g. nitrochrysenes as partly crystalline yellow solid; 0.224 g. of this solid was recrystd. to give 64% recovery of 6-nitrochrysene (IX), needles, m. 206.5-8.5° (from C2H2). The mother liquors from IX were rechromatographed to give a solid (IXa), m. 205-8°; mixed m.p. with IX depressed. The 6-position was known to be the most reactive in II; the 1-position should be the second most reactive. All other points of attack either had high reactivity numbers, or in the case of the 4- or 5-position were sterically hindered; it was suggested that IXa was 1-nitrochrysene. III (0.9 g.) was similarly nitrated and upon chromatography, 2 bands of nitro compds. were easily separated The more easily eluted band yielded 0.601 g. 6-nitrobenzo[a]pyrene (X), plates, m. 252-3°; the other band gave 0.133 g. of noncryst. material which rechromatographed and recrystd. 4 times from: C2H2 gave orange needles (XI), m. 250-2°; it was postulated that XI was either 1- or 3-nitrobenzo[a]pyrene, which had been initially contaminated by a comparable quantity of the other isomer. IV (0.248 g.) similarly nitrated and worked up gave 40 mg. V, m. 263-4° (from C6H6), which gave a red solution in H2SO4 which became green after 1 hr. at 60°; the second band gave VI, red needles, decompose at 255°, in concentrated H2SO4 which gave a red solution that did not change color, even at 200°. Examination of the other fractions failed to give positive evidence indicating whether or not any other isomer was present. In IV the 1-, 3-, and 6-positions should be of comparable reactivity. By analogy with the behavior of perylene derivs. with H2SO4, V may be 6-nitroanthanthrene. On the other hand 1- or 3-nitroanthanthrene if degraded by H2SO4 should give red solns. of the corresponding nitroanthanthrones; thus, VI was either 1- or the 3-isomer. V (10 mg.) was reduced with Pd-C and N2H4.H2O in alc. by refluxing 5 min. to give an aminoanthanthrene (XII), red needles, m. 210° (decomposition) (from C6H6). XII gave a red color in concentrated H2SO4, which rapidly became green at 30°. This also served to add to the evidence that V was 6-nitroanthanthrene. Ultraviolet absorption spectra values were given for V, VI, IX, X, XI, and XII.

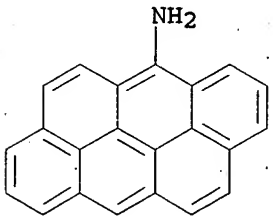
IT **111438-94-9**, Dibenzo[def,mno]chrysene, 6-nitro-
113951-46-5, Dibenzo[def,mno]chrysen-6(?)-amine
(preparation of)

RN 111438-94-9 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6-nitro- (6CI) (CA INDEX NAME)



RN 113951-46-5 HCAPLUS
CN Dibenzo[def,mno]chrysen-6-amine (6CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)
IT 86-00-0, Biphenyl, 2-nitro- 92-93-3, Biphenyl, 4-nitro- 7496-02-8, Chrysene, 6-nitro- 63041-90-7, Benzo[a]pyrene, 6-nitro- 81316-77-0, Chrysene, 1(?)-nitro- **111438-94-9**, Dibenzo[def,mno]chrysene, 6-nitro- 111614-44-9, Benzo[a]pyrene, 1(or 3)-nitro- **113951-46-5**, Dibenzo[def,mno]chrysen-6(?)-amine
(preparation of)

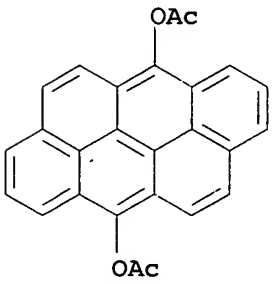
L33 ANSWER 75 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1955:42866 Document No. 49:42866 Original Reference No. 49:8233h-i,8234a-c Chemistry of anthanthrone. I. Direct replacement of hydrogen by hydroxyl and disubstituted amino groups. Bradley, Wm.; Waller, Jeffrey (Univ. Leeds, UK). Journal of the Chemical Society, Abstracts 3778-82 (Unavailable) 1953. CODEN: JCSAAZ. ISSN: 0590-9791.
AB Anthanthrone (I) [prepared by heating H2SO4 with 1,1'-binaphthyl-8,8'-dicarboxylic acid or 7,8-benzomeso-benzanthrone-3'-carboxylic acid (II), or by heating II with KOH 1 hr. at 200-20°] was characterized by reducing 1 g. suspended in H2O at 60° to 6,12-dihydroxyanthanthrene by 0.4 g. Na dithionite and 3 cc. 10% NaOH solution I (3 g.) heated 30 min. with 10 g. Zn dust and 100 cc. Ac2O gave 6,12-diacetoxyanthanthrene, yellow needles, m. 299° (decomposition) (from PhCl). I (10 g.) heated 3 hrs. at 150° with 10 g. PCl5 gave 4.1 g. hexachloro-6,12-dihydroanthanthrene, deep red needles, subliming at 325° under reduced pressure; 10 g. I stirred 1 hr. at 240° with 100 g. KOH gave 2.8 g. 3,9-dihydroxyanthanthrone (III) (di-Ac derivative, red-orange needles, m. above 360°). I (10 g.), 10 g. KClO3, and 2 g. CuCl stirred 1 hr. at 240° with 60 g. KOH gave 3.6 g. III. III (1 g.) refluxed 12 hrs. with 2 g. anhydrous K2CO3, 2 g. Me p-toluenesulfonate, and 200 cc. C6H3Cl3 gave the 3,9-di-Me ether. 1-Cyanonaphthalene-4,8-disulfonic acid (10 g.) gave 4.0 g. 5-hydroxynaphthostyril, m. above 300° [5-acetoxy-N-acetyl analog, m. 210-11° (from EtOH)]. III (10 g.) heated 3 hrs.

at 160° with 20 g. PCl5 gave tetrachloroanthanthrone, orange needles. III is strongly acidic and gives a di-Ac derivative with Ac2O and 3,6,9,12-tetraacetoxyanthanthrene with Ac2O and Zn dust, but forms no boroacetate, indicating the absence of a substituent ortho to a C:O group, and the OH groups are not replaced on heating with NH3, piperidine, or morpholine. Each C:O group of I activates 1 position in the nucleus. How marked this effect is is shown by the formation of III in the absence of an added oxidant, though the yield is higher when MnO2 or KClO3 is used.

IT **141396-66-9**, Dibenzo[cd,jk]pyrene-6,12-diol, diacetate
141396-67-0, Dibenzo[cd,jk]pyrene-6,12-diol
(preparation of)

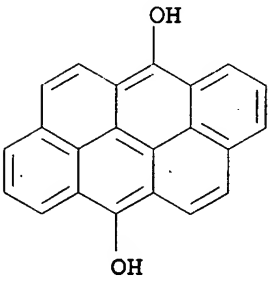
RN 141396-66-9 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, diacetate (9CI) (CA INDEX NAME)



RN 141396-67-0 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol (9CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT 641-13-4, Dibenzo[cd,jk]pyrene-6,12-dione 5507-40-4,
Naphthostyril, N-acetyl-5-hydroxy-, acetate 94734-30-2,
Naphthostyril, 5-hydroxy- **141396-66-9**,
Dibenzo[cd,jk]pyrene-6,12-diol, diacetate **141396-67-0**,
Dibenzo[cd,jk]pyrene-6,12-diol
(preparation of)

L33 ANSWER 76 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1953:15806 Document No. 47:15806 Original Reference No. 47:2739b-e
X-ray diffraction patterns of 2, 4, 7-trinitro-9-fluorenone derivatives of aromatic hydrocarbons. Hofer, L. J. E.; Peebles, W. C. (U.S. Bur. of Mines, Bruceton, PA). Anal. Chem., 24, 822-6 (Unavailable) 1952. CODEN: ANCHAM. ISSN: 0003-2700.

AB X-ray diffraction powder patterns are presented for 45 highly purified complexes of 2,4,7-trinitro-9-fluorenone (T.N.F.) and aromatic

hydrocarbons, together with m.-p. data. These complexes are those of C10H8, 1-C10H7Me, acenaphthene, fluorene, anthracene, (PhC.tplbond.)2, phenanthrene, trans-stilbene, 1,2,3,4-tetrahydroanthracene, 1,2,3,4-tetrahydrophenanthrene, 4H-cyclopenta[def]phenanthrene, 9-methylphenanthrene, fluoranthrene, pyrene, 2-C10H7Ph, 1,2-, 2,3-, and 3,4-benzofluorene, 4-methylpyrene, 2-C10H7CHPh, 1,10-trimethylphenanthrene, chrysene, 4,9-dimethylpyrene, 4-ethylpyrene, 5-, and 6-methylchrysene, benzo[k]fluoranthene, perylene, cholanthrene, (2-C10H7)2, 2-phenylphenanthrene, 5,6-dimethyl-, 5-ethyl-, and 6-ethylchrysene, naphtho[1,2-a]fluorene, 20-methylcholanthrene, 2,1-(1-C10H7)C10H6Me, dibenzo[cd, jk]pyrene, picene, 5-methylpicene, 2-C10H7Me, trans(PhCH:CH)2, periflanthene, 1,2'-binaphthyl, and T.N.F. itself. The stoichiometry of all the above complexes is 1 mol. hydrocarbon combined with 1 mol. of T.N.F. with the exception of 1,2'-binaphthyl and trans-, trans-(PhCH:CH)2, which contained 2 mols. T.N.F. and 1 of hydrocarbon. The patterns were taken with filtered FeKα radiation in 57.30 mm. and 114.59 mm. Debye Scherrer cameras. The number of spacings in the 3.1-3.5 A. interplanar spacing range is disproportionately large when compared with the interplanar spacing distribution of pure crystalline aromatic hydrocarbons (C.A. 45, 7405d). Nevertheless each pattern is unique and the method is proposed as highly reliable for pos. identification.

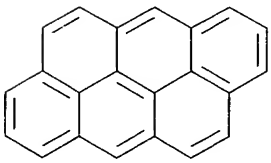
IT **96674-12-3**, Dibenzo[cd,jk]pyrene, compound with 2,4,7-trinitro-9-fluorenone
(diffraction of x-rays by)

RN 96674-12-3 HCAPLUS

CN Dibenzo[def,mno]chrysene, compd. with 2,4,7-trinitrofluoren-9-one (1:1) (7CI) (CA INDEX NAME)

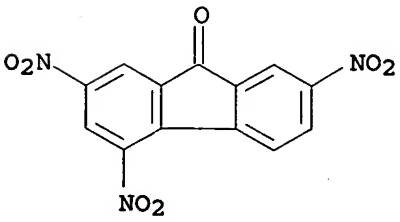
CM 1

CRN 191-26-4
CMF C22 H12



CM 2

CRN 129-79-3
CMF C13 H5 N3 O7



CC 10 (Organic Chemistry)
IT 3324-27-4, Perylene, compound with 2,4,7-trinitro-9-fluorenone
20265-02-5, Fluorene, compound with 2,4,7-trinitro-9-fluorenone
20265-03-6, Chrysene, compound with 2,4,7-trinitro-9-fluorenone
20265-14-9, Stilbene, trans-, compound with 2,4,7-trinitro-9-fluorenone 66591-49-9, Picene, compound with 2,4,7-trinitro-9-fluorenone 66591-75-1, Anthracene, 1,2,3,4-tetrahydro-, compound with 2,4,7-trinitro-9-fluorenone 66591-76-2, Picene, 5-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66903-94-4, Periflanthene, compound with 2,4,7-trinitro-9-fluorenone 66903-96-6, 13H-Naphtho[1,2-a]fluorene, compound with 2,4,7-trinitro-9-fluorenone 66907-64-0, 4H-Cyclopenta[def]phenanthrene, compound with 2,4,7-trinitro-9-fluorenone 66923-92-0, Phenanthrene, 2-phenyl-, compound with 2,4,7-trinitro-9-fluorenone 66923-93-1, Phenanthrene, 1,2,3,4-tetrahydro-, compound with 2,4,7-trinitro-9-fluorenone 66923-96-4, Chrysene, 5,6-dimethyl-, compound with 2,4,7-trinitro-9-fluorenone 66923-97-5, Chrysofluorene, compound with 2,4,7-trinitro-9-fluorenone 66923-99-7, Pyrene, 4,9-dimethyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-00-3, Cholanthrene, compound with 2,4,7-trinitro-9-fluorenone 66924-02-5, 1,2'-Binaphthyl, 1'-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-03-6, Pyrene, 4-ethyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-05-8, Cholanthrene, 3-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-07-0, Naphthalene, 1-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-07-0, Naphthalene, 1-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-08-1, Phenanthrene, 9-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-09-2, 7H-Benzo[c]fluorene, compound with 2,4,7-trinitro-9-fluorenone 66924-10-5, Pyrene, 4-methyl-, compound with 2,4,7-trinitro-9-fluorenone 66924-13-8, Fluoranthene, compound with 2,4,7-trinitro-9-fluorenone 66924-14-9, Acetylene, diphenyl-, compound with 2,4,7-trinitro-9-fluorenone **96674-12-3**, Dibenzo[cd,jk]pyrene, compound with 2,4,7-trinitro-9-fluorenone 106844-42-2, 4H-Benz[de]anthracene, 5,6-dihydro-, compound with 2,4,7-trinitro-9-fluorenone 119925-41-6, Naphthalene, 2-methyl-, compound with 2,4,7-trinitro-9-fluorenone
(diffraction of x-rays by)

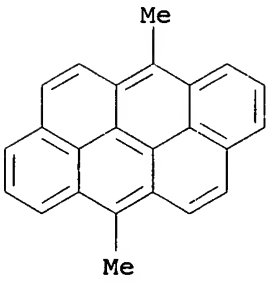
L33 ANSWER 77 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1951:41431 Document No. 45:41431 Original Reference No. 45:7095a-i
Syntheses of carcinogenic hydrocarbons. II. Martin, R. H.; Stoffyn, P. (Univ. libre, Brussels). Bulletin des Societes Chimiques Belges, 59, 208-22 (Unavailable) 1950. CODEN: BSCBAG. ISSN: 0037-9646.
GI For diagram(s), see printed CA Issue.
AB cf. C.A. 45, 598a. Two aromatic polycyclic hydrocarbons were prepared in order to test the effect of dimethylation in the meso position on the carcinogenic properties. An attempt to prepare 7,9,10,12-tetramethylbenz[a]anthracene (IA) (C.A. numbering) by condensation of β-(5,6,7,8-tetrahydro-2-naphthoyl)acrylic acid (I) and (CMe:CH2)2 (II), followed by esterification, dehydrogenation, and cyclization gave very poor yields of doubtful purity. Keto acid, C20H24O3 (III), m. 175-7°, from I and II at room temperature; its oily ester on dehydrogenation with S at 240° gave a keto ester, C21H18O3 (IV), m. 142-3.5°, cyclized by heating with concentrate H2SO4 to a mixture of 6,7-dimethyl-1,2-benzanthraquinone, m. 193°, and a very small yield of a substance m. 315°, presumably the desired isomer. Better results were obtained by condensing 1-C10H7COCH:CHCO2H with II; the keto acid, C20H20O3 (V), m. 201-3°; its oily Me ester

was dehydrogenated to the keto ester, 4,5,2-Me2(1-C10H7CO)C6H2CO2Me (VI), m. 149.5-50.5°, which was hydrolyzed to the keto acid, C20H16O3 (VII), m. 245-7°. VI or VII on cyclization with BzCl and H2SO4 gave 6,7-dimethyl-1,2-benzanthraquinone. The latter by the method of Sandin-Fieser (C.A. 35, 106.8) gave C20H20, IA, m. 129-9.5°; picrate, m. 149-50°. 7,12-Dimethylnaphtho[2,3-a]pyrene, C26H18 (VIII), m. 160-60.5° (picrate, m. 184-6°), was prepared as follows: The keto acid resulting from the condensation of pyrene with o-C6H4(CO)2O, was cyclized to 82-5% of the quinone (IX) by heating with a mixture of o-C6H4(CO)2O and BzCl and then boiling with Ac2O. IX by the method of Sandin-Fieser gave VIII. Attempts to prepare 6,12-dimethyldibenzo[cd,jk]pyrene and 9,16-dimethyltribenz[a,c,h]anthracene failed. The following condensation products which were prepared, give further proof of the structure assigned to the β-(aroyl)acrylic acids (Martin and Stoffyn, C.A. 45, 594i). Keto acid, C26H28O3, m. 246-8°, from 2-C10H7COCH:CHCO2H and 1,1'-bicyclohexen-1-yl; methyl ester, C27H30O3, m. 135-6°. Keto acid, C26H32O3, m. 219-22°, from I and 1,1'-bicyclohexen-1-yl. Keto acid, m. 190-205°, from 1-C10H7COCH:CHCO2H and bicyclohexenyl. Keto acid, C20H20O3, m. 195-6°, from 2-C10H7COCH:CHCO2H and II.

IT **41217-05-4**, Dibenzo[cd,jk]pyrene, 6,12-dimethyl- (preparation (attempted) of)

RN 41217-05-4 HCAPLUS

CN Dibenzo[def,mno]chrysene, 6,12-dimethyl- (6CI, 7CI, 9CI) (CA INDEX NAME)



CC 10 (Organic Chemistry)

IT **41217-05-4**, Dibenzo[cd,jk]pyrene, 6,12-dimethyl- (preparation (attempted) of)

L33 ANSWER 78 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1951:31259 Document No. 45:31259 Original Reference No. 45:5417d-i Leuco sulfuric esters of anthraquinone dyes. Coffey, Samuel; Fairweather, David A. W.; Hathway, David E. (Imperial Chemical Industries Ltd.). GB 633481 19490000 (Unavailable). APPLICATION: GB .

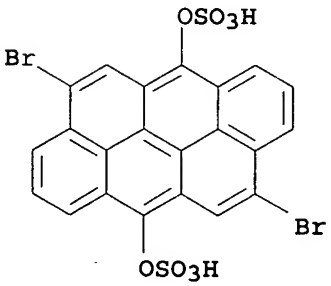
AB Leuco sulfuric esters of vat dyes and anthraquinone dye intermediates and the salts thereof are obtained by the process described above, and by using N,N-dimethylformamide (II) in the reaction mixture When II is used as the amide Zn dust is best suitable as the metal. As the catalyst in the formation of the metal salt of the leuco compound KEtSO4, Na 2-naphthol-6-sulfonate, Ca naphthalene-2,6-disulfonate, Na naphthalenesulfonate, FeCl3, or MgCl2 is used. By the above described process the following were treated: 1,4-bis(benzamido)anthraquinone (III) with Zn dust, KEtSO4,

II, and SO3) the temperature used in the first step was 50°; III is added to a mixture of MeEtCO, II, Zn dust, and Et4NBr and then heated at 80° in a N atmospheric, which is followed by sulfation at 0° as above; 16,17-dimethoxydibenzanthrone, Zn dust, Et4NBr, and II are heated at 80° in a N atmospheric and finished as before; 5,5'-diethoxythioindigo, Zn dust, KEtSO4, and II are heated at 80° in N and sulfated with a solution of SO3 in II as before; 2-(1-amino-2-anthraquinonyl)anthraquinone-2',3'-oxazole, KMeSO4, Zn dust, and II are heated at 80-100° and then cooled to 0°, followed by sulfation with a mixture of Me chlorosulfonate in II and finished as before; 3-chloro-2-acetamidoanthraquinone, II, Zn dust, and Et4NBr are heated at 35° in N, and sulfated with SO3 in II; 2-chloroanthraquinone, Zn dust, crystalline MgCl2, and II are heated at 40° in N, sulfated with a mixture of Me chlorosulfonate in II, and finished as before; anthraquinone, Zn dust, Na 2-naphthalenesulfonate, and II are heated at 60° in N and sulfated as in the preceding example; and anthraquinone, Zn dust, Et4NBr, and N-methylformanilide (IV) are heated at 80° in N and then sulfated with Me chlorosulfonate in IV at 0°. In 15 more quoted expts. the above and other difficultly reducible vat dyes, i.e. 9,10-dihydroxyanthracene, leucoindigo, 4,10-dibromoanthrathrone, 1,1',4,1''-trianthrimide-2,2',3,2''-dicarbazole, 1-anthraquinonylurethane, 1,1'-dianthrimide, and leucoflavanthrone, are subjected to treatment with II-SO3 or its equivalent as above at temps. below 80° to give the desired leuco sulfuric esters.

IT **4378-58-9**, Dibenzo[cd,jk]pyrene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate)
(preparation of)

RN 4378-58-9 HCAPLUS

CN Dibenzo[def,mno]chrysene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) (8CI, 9CI) (CA INDEX NAME)



CC 25 (Dyes and Textiles Chemistry)

IT 117-63-5, Acetamide, N-(3-chloro-9,10-dihydroxy-2-anthryl)-, bis(hydrogen sulfate) 2678-71-9, Dinaphtho[1,2,3-cd,3',2',1'-lm]perylene-5,10-diol, 16,17-dimethoxy-, bis(hydrogen sulfate) **4378-58-9**, Dibenzo[cd,jk]pyrene-6,12-diol, 4,10-dibromo-, bis(hydrogen sulfate) 121600-14-4, Benzamide, N,N'-(9,10-dihydroxy-1,4-anthrylene)bis-, bis(hydrogen sulfate)
(preparation of)

L33 ANSWER 79 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1950:50694 Document No. 44:50694 Original Reference No. 44:9688e-i,9689a-e Sulfur colors. Robbins, Gordon B. (E. I. du Pont de Nemours & Co.). US 2504153 19500418 (Unavailable). APPLICATION: US .

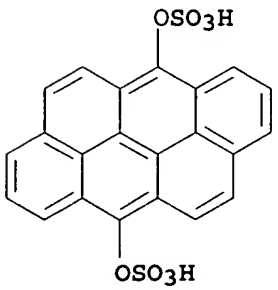
GI For diagram(s), see printed CA Issue.

AB Violet to red sulfur colors are prepared by treating triphenodioxazine pigments with the complex agent (I) resulting from the fusion of AlCl3 with S2Cl2. The general type formula (A) of the dioxazine compds., where X is H, halogen, or alkyl and Ar designates aromatic radicals such as the benzene, naphthalene, fluorenone, carbazole or furan groups, may be thus treated. The new compds. are assumed to contain disulfide groups, which are reduced by the alkaline sulfide vat to mercapto groups. I is prepared by heating S2Cl2 162 and AlCl3 80 parts at 80-100° for several hrs. A red-violet cotton dye is prepared by heating 6,13-dichlorotriphenodioxazine 1 (prepared by ring-closure of the diarylaminoquinone from o-anisidine and chloranil in PhNO2 with the aid of PhCOCl) with I 17.5 at 120°. The mixture is drowned in ice water 100 containing HCl 5 and stirred to decompose excess of I. The filtered material is extracted with H2O 150 at 80-90°. NaOH is added until most of the excess S compds. have dissolved. The dye is filtered, washed neutral, and dried. The product can be vatted and dyed with Na2S by usual methods. Other triphenodioxazine pigments are prepared similarly. In each case cited below the dioxazine formula is followed by the amine used with chloranil in forming the diarylaminoquinone: 3,6,10,13-tetrachlorotriphenodioxazine from 2-methoxy-15-chloroaniline (II); 2,6,9,13-tetrachlorotri phenodioxazine from p-chloroaniline; 1,4,6,8,11,13-hexachlorotriphenodioxazine, from 2,5-dichloroaniline; 3,10-dimethyl-6,13-dichlorotriphenodioxazine from 2-methoxy-5-methylaniline; 2,9-diphenyl-6,13-dichlorotriphenodioxazine from 4-aminobiphenyl (III); 3,10-diphenyl-6,13-dichlorotriphenodioxazine from 3-amino-4-methoxybiphenyl; 2,9-bis(p-bromophenyl)-6,13-dichlorotriphenodioxazine from 4-amino-4'-bromobiphenyl; 2,9-dibenzoyl-6,13-dichlorotriphenodioxazine from 4-aminobenzophenone; 2,9-bis(p-acetamido-m-methoxyphenyl)-6,13-dichlorotriphenodioxazine from monoacetyldianisidine; 3,10-dimethoxy-6,13-dichlorotriphenodioxazine from 2,5-dimethoxyaniline; 2,9-diphenoxy-6,13-dichlorotriphenodioxazine from 4-aminodiphenyloxide; 3,10-dichlorotriphenodioxazine from II; 2,9-diphenyl-6,13-dibromotriphenodioxazine from III (but using bromanil instead of chloranil); a dioxazine (IV) (IVa, A = CO, X = Cl) from 2-aminofluorenone; V from 3-aminocarbazole; VI (IVa, A = O, X = Cl) from 3-aminodibenzofuran (VII); VIII (IVa, A = O, X = Br) from VII (but using bromanil instead of chloranil).

IT **114305-70-3**, Dibenzo[cd,jk]pyrene-6,12-diol, bis(hydrogen sulfate)
(preparation of)

RN 114305-70-3 HCAPLUS

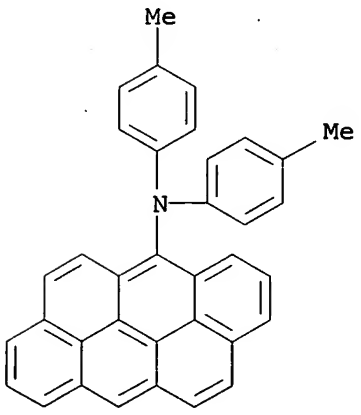
CN Dibenzo[def,mno]chrysen-6,12-ylene sulfate (6CI) (CA INDEX NAME)



CC 25 (Dyes and Textiles Chemistry)
IT 4794-44-9, Triphenodioxazine, 6,13-dichloro- 4794-50-7, Triphenodioxazine, 6,13-dichloro-2,9-dimethyl- 5174-20-9, Triphenodioxazine, 6,13-dichloro-2,9-dimethoxy- 6252-81-9, Dibenzo[a,h]pyrene-7,14-diol, bis(hydrogen sulfate) 13437-05-3, Triphenodioxazine, 6,13-dichloro-3,10-diphenyl- 13437-06-4, Triphenodioxazine, 6,13-dichloro-2,9-diphenyl- 13437-07-5, Triphenodioxazine, 3,6,10,13-tetrachloro- 13437-45-1, Triphenodioxazine, 3,10-bis(p-bromophenyl)-6,13-dichloro- 17222-30-9, Triphenodioxazine, 2,6,9,13-tetrachloro- 32577-45-0, Triphenodioxazine, 3,10-bis(4-acetamido-3-methoxyphenyl)-6,13-dichloro- 32577-50-7, Triphenodioxazine, 6,13-dichloro-3,10-diphenoxy- 52829-20-6, Triphenodioxazine, 2,9-dichloro- 88318-66-5, Diindolo[3,2-b,3',2'-m]triphenodioxazine, 8,18-dichloro-5,15-dihydro- 103006-00-4, Triphenodioxazine, 3,10-dibenzoyl-6,13-dichloro- **114305-70-3**, Dibenzo[cd,jk]pyrene-6,12-diol, bis(hydrogen sulfate) 167647-25-8, Triphenodioxazine, 1,4,6,8,11,13-hexachloro-
(preparation of)

=> d l33 3,9,17,23,25 cbib fhitstr

L33 ANSWER 3 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2003:317922 Document No. 138:347368 High electron-mobility and high ON/OFF-current-ratio organic thin-film transistors. Higashiguchi, Itaru; Oda, Atsushi; Ishikawa, Hitoshi (NEC Corp., Japan). Jpn. Kokai Tokkyo Koho JP 2003124472 A2 20030425, 77 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 2001-320342 20011018.
IT **515833-07-5**
RL: DEV (Device component use); PRP (Properties); TEM (Technical or engineered material use); USES (Uses)
(high electron-mobility and high ON/OFF-current-ratio organic aromatic-heterocyclic compound thin-film transistors)
RN 515833-07-5 HCAPLUS
CN Dibenzo[def,mno]chrysen-6-amine, N,N-bis(4-methylphenyl)- (9CI) (CA INDEX NAME)



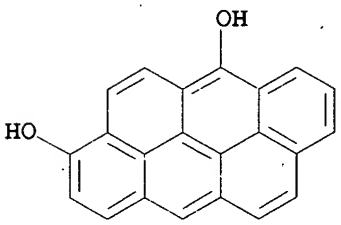
L33 ANSWER 9 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
2002:96307 Document No. 136:195529 Microsomal Activation of

Dibenzo[def,mno]chrysene (Anthanthrene), a Hexacyclic Aromatic Hydrocarbon without a Bay-Region, to Mutagenic Metabolites. Platt, Karl L.; Degenhardt, Christian; Grupe, Stefanie; Frank, Heinz; Seidel, Albrecht (Institute of Toxicology, University of Mainz, Mainz, D-55131, Germany). Chemical Research in Toxicology, 15(3), 332-342 (English) 2002. CODEN: CRTOEC. ISSN: 0893-228X. Publisher: American Chemical Society.

IT **400778-35-0**, Dibenzo[def,mno]chrysene-3,6-diol
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)
(microsomal activation of dibenzochrysene to mutagenic metabolites)

RN 400778-35-0 HCAPLUS

CN Dibenzo[def,mno]chrysene-3,6-diol (9CI) (CA INDEX NAME)



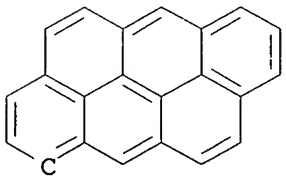
L33 ANSWER 17 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

1996:677901 Document No. 125:327779 The C-H bond dissociation energies of polycyclic aromatic hydrocarbons. Aihara, Jun-ichi; Fujiwara, Kenji; Harada, Akinori; Ichikawa, Hiroshi; Fukushima, Kunio; Hirota, Fumihiko; Ishida, Toshimasa (Department of Chemistry, Shizuoka University, Shuzuoka, 422, Japan). THEOCHEM, 366(3), 219-226 (English) 1996. CODEN: THEODJ. ISSN: 0166-1280. Publisher: Elsevier.

IT **183321-92-8**, Dibenzo[def,mno]chrysen-1-yl
RL: PRP (Properties)
(PM3 MO calcns. of C-H bond dissociation energies of polycyclic aromatic hydrocarbons)

RN 183321-92-8 HCAPLUS

CN Dibenzo[def,mno]chrysen-1-yl (9CI) (CA INDEX NAME)

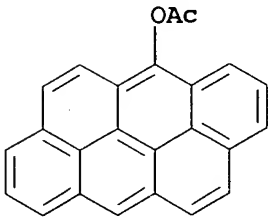


L33 ANSWER 23 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN

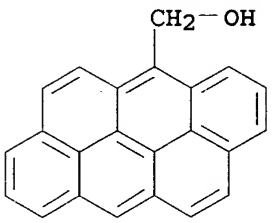
1992:250195 Document No. 116:250195 One-electron oxidation of dibenzo[a]pyrenes by manganic acetate. Cremonesi, Paolo; Hietbrink, Bruce; Rogan, Eleanor G.; Cavalieri, Ercole L. (Eppley Inst. Res. Cancer Allied dis., Omaha, NE, 68198-6805, USA). Journal of Organic Chemistry, 57(12), 3309-12 (English) 1992. CODEN: JOCEAH. ISSN: 0022-3263.

IT **141396-65-8**

RL: BIOL (Biological study)
(as anthracene-oxidation product, after manganic acetate treatment)
RN 141396-65-8 HCAPLUS
CN Dibenzo[def,mno]chrysen-6-ol, acetate (9CI) (CA INDEX NAME)



L33 ANSWER 25 OF 79 HCAPLUS COPYRIGHT 2005 ACS on STN
1987:14437 Document No. 106:14437 Mutagenicity of benzylic acetates, sulfates and bromides of polycyclic aromatic hydrocarbons. Rogan, Eleanor G.; Cavalieri, Ercole L.; Walker, Betty A.; Balasubramanian, Ramadas; Wislocki, Peter G.; Roth, Robert W.; Saugier, Richard K. (Med. Cent., Univ. Nebraska, Omaha, NE, 68105, USA). Chemico-Biological Interactions, 58(3), 253-75 (English) 1986. CODEN: CBINA8. ISSN: 0009-2797.
IT **105708-72-3**
RL: PROC (Process)
(acetylation or bromide substitution of)
RN 105708-72-3 HCAPLUS
CN Dibenzo[def,mno]chrysene-6-methanol (9CI) (CA INDEX NAME)



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